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EXPERIMENTS AND MODELING OF MULTI-COMPONENT FUEL BEHAVIOR IN COMBUSTION

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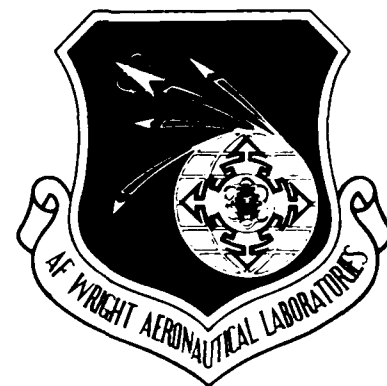James R. Markham

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)
A computer model was developed to relate pyrolysis and soot formation to fuel properties. A Fourier Transform-Infrared Spectrometer (FT-IR) was used to characterize the effect of temperature, pressure, reaction time, and hydrogen and oxygen concentration of fuels undergoing pyrolysis. The problem of how to identify and measure the hydrogen available for release during pyrolysis was investigated. A detailed data base of a variety of fuels undergoing pyrolysis was developed. The data base conditions included: temperature 800-1500°C; pressure 1-15 atm; and reaction time 100ms-1 sec. Experimental data results show that fuels decompose to form small hydrocarbon species prior to the onset of soot formation. A hydrocarbon model was extended to include Rice-Kossiakoff-Herzfeld mechanism to predict the decomposition of long chain aliphatics to small molecules. A free radical soot model was developed to predict the growth of soot precursors from the small molecules.

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SUMMARY

An experimental and theoretical program has been performed to develop a database and modeling capabilities to relate pyrolysis and soot formation to the properties of the fuel. The method of approach to studying soot formation was to perform well-instrumented studies using FT-IR under pyrolysis conditions where variables such as temperature, pressure, reaction time and hydrogen or oxygen concentration were varied and controlled. The problem is to provide fuel specification, fuel processing strategies and combustion design concepts to reduce soot, but which still allow utilization of readily available fuels. **While many trends have been established, there is no accepted model for soot formation.**

Based on the Phase I results, it appeared that the "hydrogen available for release" in pyrolysis controls soot production. A major focus of the program was to identify how this parameter can be measured, the mechanisms by which it affects soot production and to develop methods based on these mechanisms for controlling soot.

Key accomplishments in this program were: A data base of detailed pyrolysis measurements on a large number of fuels, including several high density, aromatic fuels has been created. Temperature varied from 800°C to 1500°C, pressures from 1 to 15 atm and residence times from 100 ms to 1 sec. A key conclusion of Task I was that in almost all cases at one atmosphere the fuels decomposed to form a limited number of small species prior to the onset of sooting. The aliphatic portion of the fuels formed H_2, C_1's, and C_2's. The aromatic portion of the fuels formed benzene, 2-ring and possibly 3-ring aromatics. This is a significant result and justifies our approach to modeling the sooting tendencies of complex fuels based on a limited number of small species.

The measurements of radiance for these fuels showed factors of two or three variation for comparable amounts of soot. The causes of this are probably due to soot age (H/C content) which would change the optical constants for the soot, or soot particle size. This observation is significant for heat transfer from the soot in combustion, and for its impact on the soot signature left by an engine. In all cases, we found that the addition of small amounts of hydrogen (as H_2) reduced the soot while similar amounts of O_2 increased it.

In Task II, a factor analysis correlation was performed which showed that the complex IR spectra of the hydrocarbon could be characterized by a few factors which could be used to predict the combustion properties of the fuels, for example, the sooting as measured in Task I, or the smoke point as measured by standard techniques.

The hydrocarbon cracking model began in Phase I was extended using a modified Rice-Kossiakoff-Herzfeld (RKH) mechanism. This model predicts the decomposition of long chain aliphatics into small molecules, (C_2H_2, C_2H_4, H_2). A soot model based on published free radical mechanisms and rates was implemented on AFR's Sun 3/260 workstation and used to predict the growth of the soot precursors from the small molecules produced.

A heat transfer model was developed to provide the temperature-time profiles required by both models. The combination of these models can predict not only the soot, but also the intermediate light species of pyrolysis (C_2's, C_3's, C_4's, light aromatics) to within a factor of two.

ACKNOWLEDGEMENTS

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I. INTRODUCTION

The objectives of this program are to develop a database and modeling capabilities to relate pyrolysis and soot formation to the properties of the fuel. The method of approach to studying soot formation is to perform well-instrumented studies under pyrolysis conditions where variables such as temperature, pressure, reaction time and hydrogen or oxygen concentration can be varied and controlled. Pyrolysis is a suitable tool for investigating the sooting because, as suggested by many investigators, soot growth is controlled by the pyrolysis rate and occurs in the pyrolysis zone of flames. The experiments at zero or low oxygen concentrations allow the study of soot growth without the complication of soot precursor destruction or the consumption of hydrogen by oxidation. Without the complications introduced by a flame, it is possible to perform more easily interpreted experiments to study chemical reaction pathways. A series of these experiments has been performed to test this concept that soot growth occurs via formation of thermodynamically stable intermediate Poly-Aromatic Hydrocarbons (PAH's). In particular, we have tested the effect of hydrogen concentration on soot formation by systematic experiments which include the addition of hydrogen.

The method of approach to characterize the fuel by Fourier Transform Infrared (FT-IR) is a useful one because it measures the functional groups present in the fuels, as opposed to the more customary wet chemical techniques which just determine the fraction of aromatics, olefins, and paraffins. In the standard methods, aliphatics attached to aromatic groups are reported as aromatic. For soot chemistry, these attached groups will behave as aliphatics. The FT-IR functional group determinations eliminate this problem and are useful because from this information one can predict the initial cracking of the fuels into the small fragments which are important for soot formation.

The original proposal included tasks for vaporization and droplet studies with characterization of multi-component fuel sprays, but the multi-component spray studies were eliminated in the original contract and the droplet vaporization was replaced by prevaporized fuel in the contract redirection. This report describes the Phase II study which addressed the above objectives in four tasks (numbered I, II, IV and V to agree with the numbering in the proposal and contract documents).

The remainder of this section provides a summary of the program. This includes a description of the problems being addressed, the methodology used to

approach these problems, and a summary of the goals and accomplishments of this program.

Section II presents a description of the experimental facilities and procedures. Section III presents the detailed results by task, and Section IV presents the results, conclusions, and recommendations.

Objective

An important Air Force objective is to develop technology to allow the utilization of aviation fuels with a broader range of properties including lower hydrogen content and higher aromaticity. Such fuels, will be increasingly important as the sources shift to heavier petroleum, oil shale, tar sands, and coal derived fuels. The combustion of such fuels adds substantial complexities to fuel volatilization and pyrolysis, and increases the potential for higher radiative emission from soot, reducing the useful life of turbine combustors. Also, the smoke emitted from an engine, resulting from unburned soot, is both a pollutant and a problem due to increased visibility for detecting and targeting of military aircraft.

Current research suggests that the sooting potential of an aircraft fuel increases with decrease in hydrogen or alternatively, increases with increasing aromatic content. The problem is, therefore, to provide fuel specification, fuel processing strategies and combustion design concepts to reduce soot, but which still allow utilization of readily available fuels. **While many trends have been established, there is no accepted model for soot formation.**

Methodology

The objectives of this program are to develop a database and modeling capabilities to relate pyrolysis and soot formation to the properties of the fuel and combustion conditions. It is soot generation and its radiation which appears to be the major problem. Based on the Phase I results, it appeared that the "hydrogen available for release" in pyrolysis controls soot production. A major focus of the program is to identify how this parameter can be measured, the mechanisms by which it affects soot production and methods based on these mechanisms for controlling soot.

Task I addressed the mechanistic studies of pyrolysis and soot formation, and

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was the main experimental task. In this task, data were obtained on 37 hydrocarbon fuels. The data include complete mass balances, and full emission/transmission spectra (500 cm^{-1} to 6500 cm^{-1}) for several temperatures (1100°C to 1500°C) and for various pyrolysis times (100 ms to 700 ms). The mass balance experiments determine the light species (C_2H_2, C_2H_4, CH_4, paraffins, olefins) by FT-IR, H_2, benzene, and heavier hydrocarbons by GC, and tar and soot gravimetrically. Several of the experiments were performed with added H_2 or O_2. The data base also includes room temperature liquid characterization by FT-IR.

The fuels analyzed included the 25 fuels from a NASA study provided by the Air Force, plus the four JP8X's, also provided by the Air Force. The 25 fuels from NASA were selected and blended by NASA and UTRC to provide a range of naphthalene, hydrogen, and total aromatic content. In addition, pure hydrocarbons (benzene, butane, acetylene, and dodecane) were included.

Task II was the study of the characterization of the fuel using the FT-IR spectra of the liquid fuels and included extensive correlations of the spectral features with the sooting behavior measured in Task I as well as correlation with literature data.

Task IV addressed the development of a general fuel pyrolysis model to correlate pyrolysis behavior with fuel properties. The model includes three submodels: a hydrocarbon cracking model, a soot production model, and a heat transfer model which provides the time-temperature profiles required by the chemistry submodels.

Task V studied the effect of pressure on the pyrolysis of several of the fuels.

Results

- A data base of detailed pyrolysis measurements on a large number of fuels, including several high density, aromatic fuels has been created. Temperature varied from 800°C to 1500°C, pressures from 1 to 15 atm and residence times from 100 ms to 1 sec.

- A key conclusion of Task I is that in almost all cases at one atmosphere the fuels have decomposed to form a limited number of small species prior to the onset of sooting. The aliphatic portion of the fuels formed

H_2, C_1's, and C_2's. The aromatic portion of the fuels formed benzene, 2-ring and possibly 3-ring aromatics. This is a significant result and justifies our approach to modeling the sooting tendencies of complex fuels based on a limited number of small species, since the fuels all crack to these starting fragments prior to soot formation.

- The measurements of radiance for these fuels show factors of two or three variation for comparable amounts of soot. The causes of this are probably due to soot age (H/C content) which would change the optical constants for the soot or soot particle size. This observation is significant for heat transfer from the soot in combustion, and for its impact on the soot signature left by an engine.

- In all cases, we find that the addition of small amounts of hydrogen (as H_2) reduces the soot while similar amounts of O_2 increase it. This again has significance for the soot signature of a jet engine. One can imagine adding a pulse of H_2 to reduce the IR signature under emergency conditions.

- In Task II, a factor analysis correlation was performed which shows that the complex IR spectra of the hydrocarbon can be characterized by a few (10) factors which can reproduce the spectra to within 5%. Secondly, these factors can be used to predict the combustion properties of the fuels, in particular the sooting as measured in Task I, or the smoke point as measured by standard techniques.

- The hydrocarbon cracking model began in Phase I was extended using a modified Rice-Kossiakoff-Herzfeld (RKH) mechanism. This model predicts the decomposition of long chain aliphatics into small molecules, (C_2H_2, C_2H_4, H_2).

- A soot model based on published free radical mechanisms and rates was implemented on AFR's Sun 3/260 workstation and used to predict the growth of the soot precursors from the small molecules produced.

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- The combination of these models can predict not only the soot, but also the intermediate light species of pyrolysis (C_2's, C_3's, C_4's, light aromatics) to within a factor of two.

Papers Supported by this Program

"A Kinetic Model for the Pyrolysis of Large N-Alkanes," Kevin R. Squire, Michael A. Serio, Peter R. Solomon, and David G. Hamblen, to be submitted to Combustion and Flame (1987).

"FT-IR Emission/Transmission Spectroscopy for In-Situ Combustion Diagnostics," Peter R. Solomon, Philip E. Best, Robert M. Carangelo, James R. Markham, P.L. Chien, Robert J. Santoro, and H.G. Semerjian, 21st Symposium (Int) on Combustion, the Combustion Institute, Pittsburgh, PA, (in press) (1987).

"Correlations Between Fuel Structure and Soot Potential," David G. Hamblen, Peter R. Solomon, Kenneth S. Tarantul, and Robert M. Carangelo, presented at the ACS Meeting, Div. of Petroleum Chemistry, Denver, CO, (1987).

"Pressure Effects in Pyrolysis of Large N-Alkanes," Michael A. Serio, Peter R. Solomon, David G. Hamblen, and Kevin R. Squire, presented at the ACS Meeting, Symposium on Chemical and Mechanical Modeling of Complex Reaction Systems, Anaheim, CA, (1986).

II. EXPERIMENTAL

The objective of Task I, Mechanistic Studies of Pyrolysis, Combustion, and Soot Production, was to measure and develop an understanding of the pyrolysis, combustion and soot production from a variety of liquid fuels. The main experimental facility used was AFR's entrained flow reactor (EFR). The fuel injection system was modified to provide fuel in vapor form. The fuels and products were analyzed using a variety of techniques including Fourier Transform Infrared Spectroscopy (FT-IR), GC, Field Ionization Mass Spectroscopy (FIMS), and AFR's Evolved Gas/Thermogravimetric Analyzer (EGA/TGA). In this section, we describe the experimental facilities used. The experimental results will be presented in Section III, Task I.

Entrained Flow Reactor

The entrained flow reactor is shown in Fig. 1. It employs a Nicolet 7199 FT-IR for in-situ analysis of gas species and gas temperature and quantitative analysis of the gas composition after cooling. To operate the reactor, a gas stream of predetermined composition is heated during transit through the heat exchanger (maintained at furnace temperature). The gas stream then turns through the U-tube and enters a 5 cm diameter test section, maintained at the furnace temperature. Fuel was introduced into the test section at variable positions through a movable heated injector which allows samples to be injected at any position along the center line of a 75 cm long, 50.8 mm i.d. hot alumina tube in which the preheated gas is flowing. There is a continuous drop in temperature over the bottom 35 cm which was designed for optical access, and does not receive direct radiation from the elements. Details of the temperature profiles are presented with the modeling results (see Figs. 72-74). After a variable residence time, the reacting stream passes optical access ports and immediately downstream, is quenched in a water cooled collector. Two optical access ports are employed for the FT-IR beam.

The hot injector is shown in Fig. 2. It consists of a liquid jacketed moveable injector, with a pump to circulate the coolant (Dow Therm A) through the injector. The fluid reservoir is thermostatically controlled with heating tapes and a water-cooled coil. The coolant through the injector can be switched to water in the event of pump failure in order to protect the injector. During experimental runs, the injector tip is maintained at approximately 250°C as measured with a thermocouple. This is sufficient to vaporize most of the fuels.

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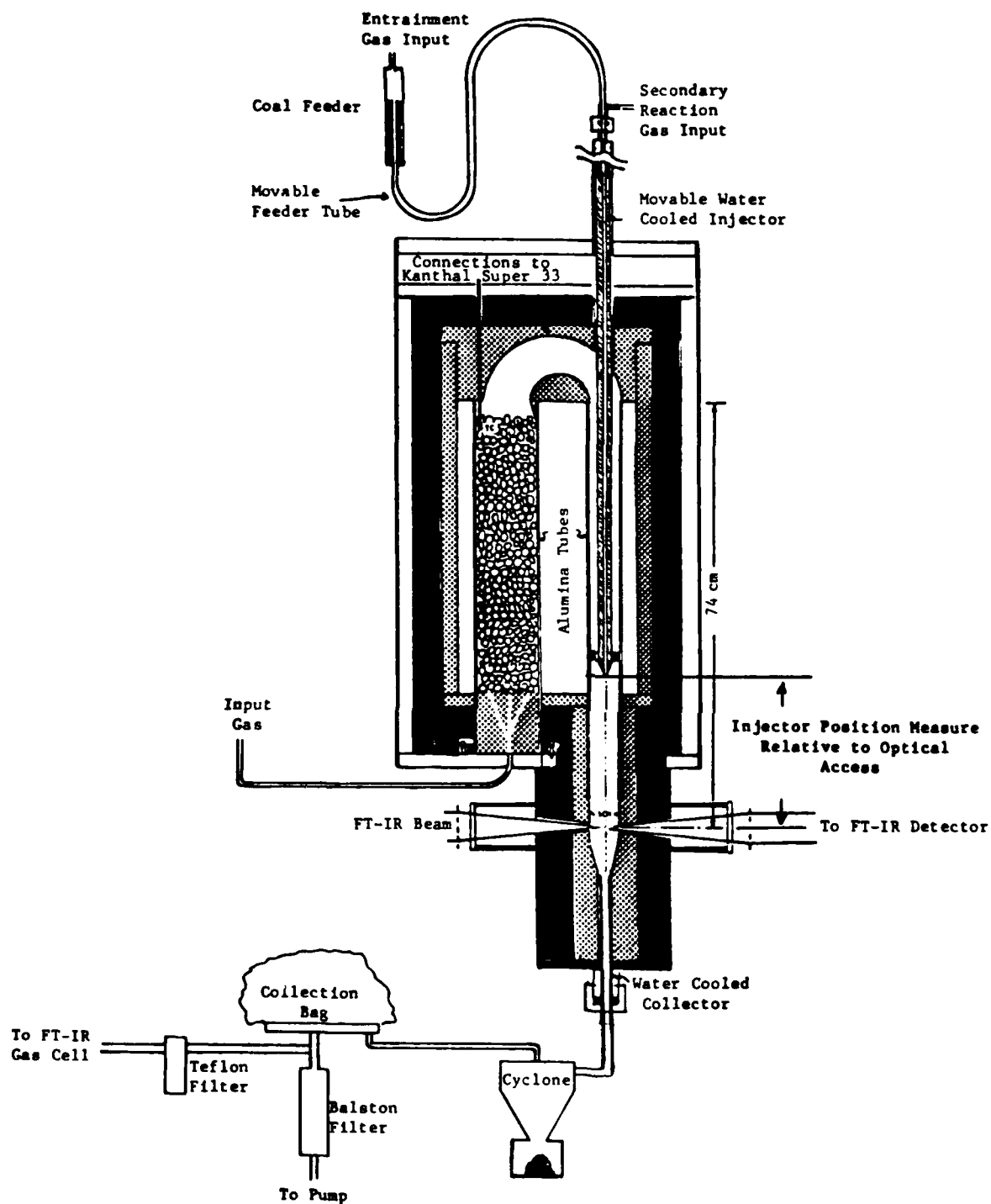
Figure 1. Schematic of Entrained Flow Reactor.
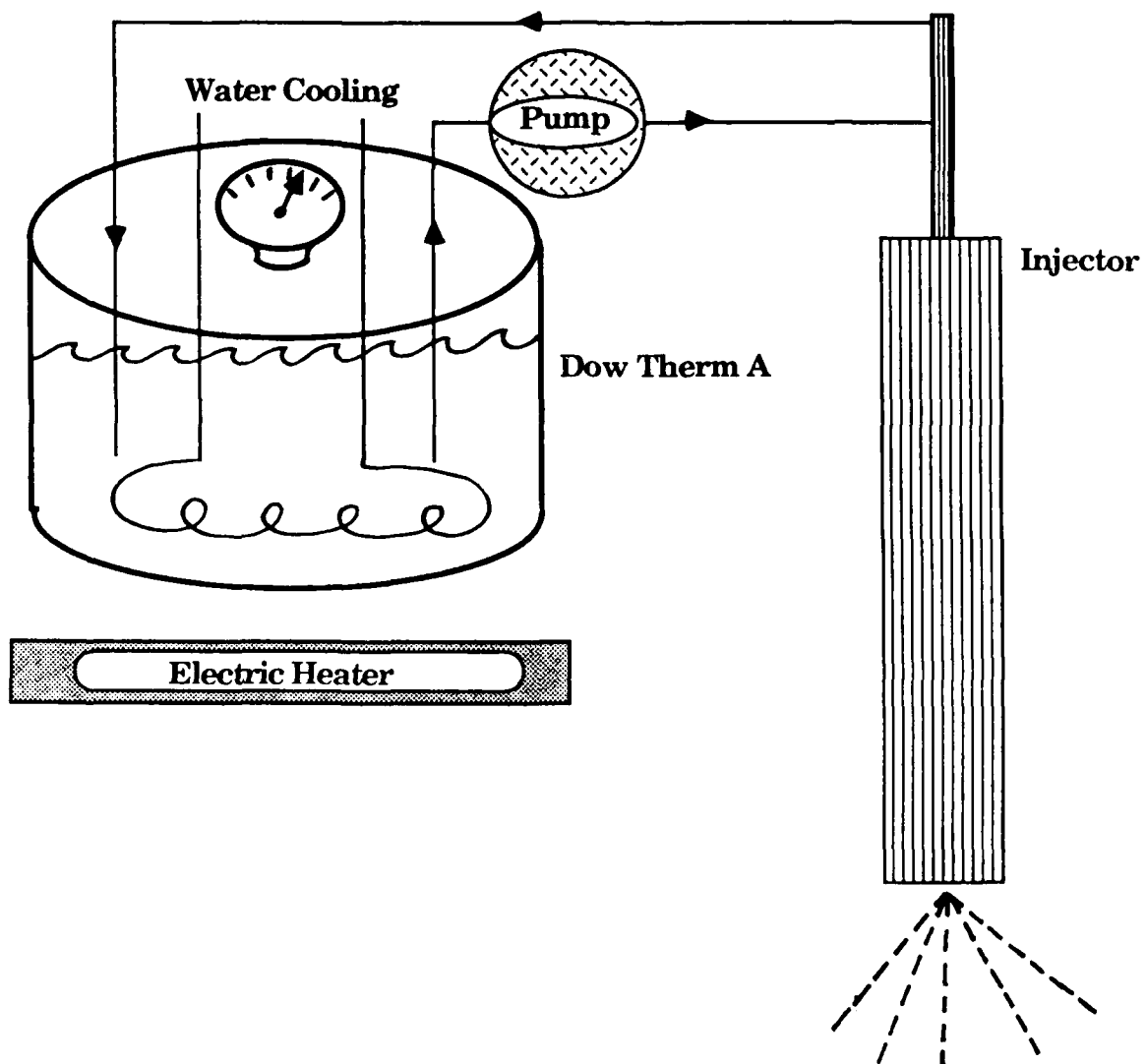
Figure 2. Schematic Diagram of Hot Injector.

The fuel injection system consists of a syringe pump connected to the moveable injector by flexible stainless steel hypo tubing (0.032" I.D.). The tip of the injector is a short piece of small (0.010" dia) hypo tubing which is small enough to prevent dripping when the pump is shut off.

The hot injector position was positioned daily in order to ensure that the infrared beam would see the center of the soot stream in the reactor (i.e. maximum beam blockage). This was done by moving the injector radially while a standard fuel (ERBS) flowed into the reactor, and observing the IR beam intensity.

Fuel flow rates were maintained at 1.2 ml/min. The fuel was filtered before use to prevent particulate contaminants from plugging the small i.d. hypotubing used for sample delivery. Bubbling nitrogen through the fuel in order to remove dissolved oxygen or other gases seemed not to make a difference in experimental results. Therefore, this practice, which had been maintained through the mass balance experiments, was discontinued for the emission/transmission experiments.

The sample collection and analysis system consists of a water-cooled extractor, to quench the reactions, which feeds a 100 liter polyethylene bag through a cyclone which removes particles larger than 5 μm. This bag is large enough to hold the full exhaust of the reactor during a 3 minute experimental run, and serves to smooth out any fluctuations in the fuel feed rate. The volume of the bag is measured at the end of the run, a sample of gas is extracted into the FTIR cell for gas analysis; another sample is extracted for GC analysis to determine H_2, benzene, and some of the heavier aliphatics. The bag is then evacuated through a Balston filter, to collect any entrained tars or soot. The weight gains of the bag, the aluminum foil liner of the bag holder and the filter are measured and reported as tar. The extractor, the cyclone, and the associated plumbing are rinsed with acetone, and the products filtered and dried. The solids in the filter are reported as soot (or char) and the acetone-soluble fraction is reported as tar. Mass balances are usually between 90 to 110% of the input fuel.

The FT-IR allows data to be obtained on gas composition and temperature as previously discussed by us (1,2) and others (3-5).

Figure 3 compares the spectra from the in-situ analysis and room temperature gas cell analysis for the furnace at 1100°C. In transmission measurements, radiation from a globar source passes through the interferometer before traversing the reactor to the detector. In passage through the interferometer the radiation

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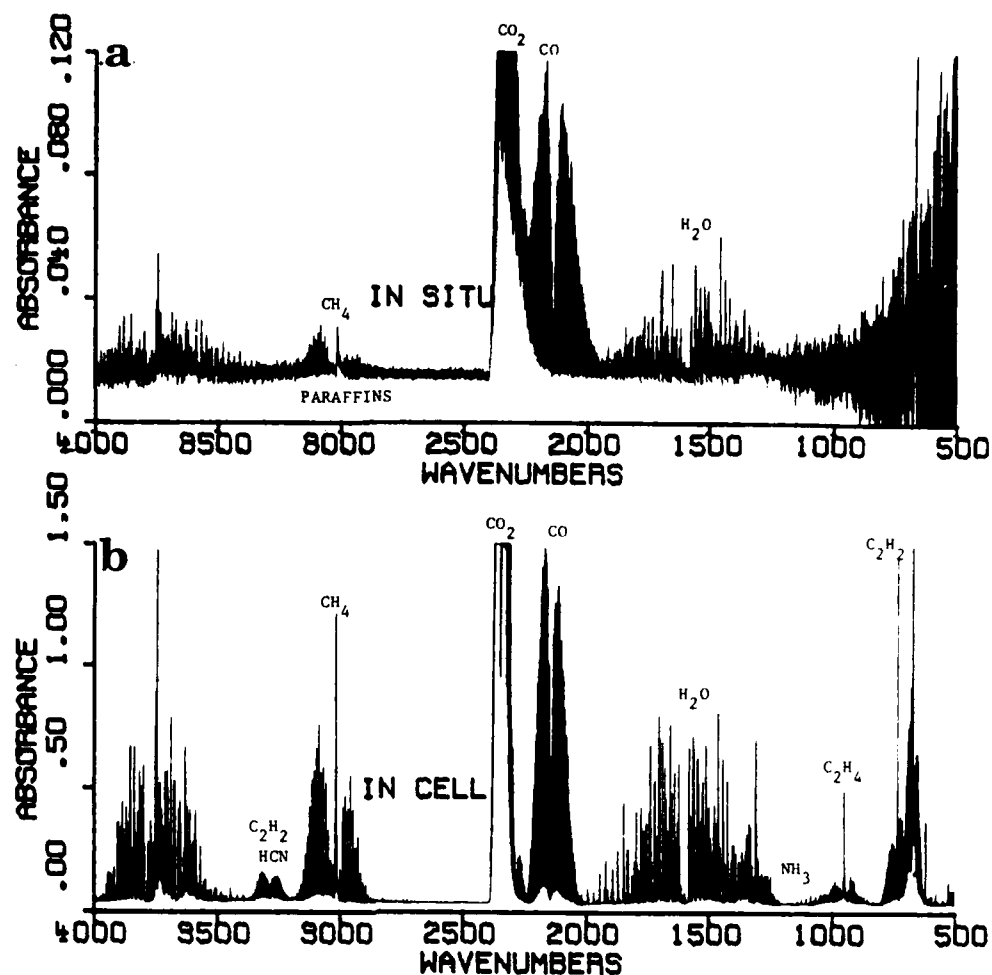
Figure 3. FT-IR Spectra of Pyrolysis Gases from Beulah, North Dakota Lignite at 1100°C. a) In-situ Spectrum and b) Room Temperature Cell Spectrum.
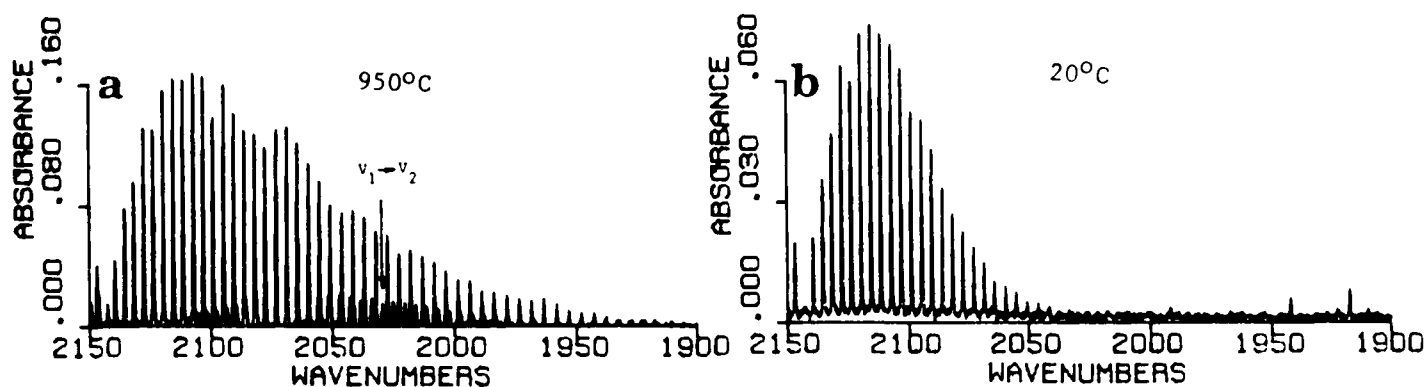
Figure 4. Spectra of Carbon Monoxide in Furnace at 950°C and 20°C.

is amplitude modulated as a function of wavelength, and it is only modulated radiation that is detected. In this way the transmission experiment measures the extinction, independent of emission from the furnace. Easily seen in the hot spectrum are CO, CO_2, H_2O, CH_4, and heavy paraffins. The lower noise of the room temperature spectrum permits the measurement of additional species including C_2H_2, C_2H_4, C_2H_6, C_3H_6, HCN, NH_3, COS, CS_2, SO_2, and heavy paraffins. This spectrum is used for quantitative analysis. A typical gas analysis together with the yield of solids and liquids is presented in Table 1.

The relative intensities of the hot CO absorption lines can be used for measuring gas temperature (1). Figure 4 compares the in-situ CO spectra at measured furnace temperatures of 20°C and 950°C; the calculated temperatures from line intensities are 30°C and 1050°C.

Temperatures and Soot Concentrations by FT-IR Emission/Transmission (E/T) Spectroscopy

Introduction

In investigating the behavior of combusting systems, it is desirable to have non-intrusive techniques to monitor the composition, physical properties and temperature of the various phases (gas, soot particles, droplets, aerosols, coal, char, and fly ash) present. Laser spectroscopic and scattering techniques, as well as other optical diagnostics have been developed for gas species concentration, gas temperature and particle properties. Many of these techniques were recently reviewed by Penner, et al. (6,7) and Hardesty (8). Advances in optical emission techniques to measure size, velocity, and temperature of single particles have also been reported (9,10).

Among the methods which have been employed, Fourier Transform Infrared (FT-IR) Spectroscopy has shown promise as a versatile technique. In addition to the FT-IR Transmission Spectroscopy discussed above to determine both gas concentrations and temperatures, we have recently implemented an infrared emission/transmission (E/T) technique, (a method previously applied to gases (11-13) and soot particles (14) using dispersive infrared) using the FT-IR spectrometer. The full description for gases and soot are presented in Ref. 15.

FT-IR Instrument - The apparatus employed in the experiments consists of a FT-IR spectrometer coupled to the entrained flow reactor, such that the FT-IR beam

TABLE 1 - Typical Gas Master.

RUN CONDITIONS

2490.50 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid.
763.120 mm. Final Pressure for 86.7060 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 8 - 14 - 86   13 : 48
Stored => 9 - 22 - 86   8 : 0

UTRC 2A
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	42.5697
Tar	6.25175
Gas	37.8807
Water	1.34835
Missing	11.9494

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	9.44388	.40622	7.08291	2.36097	0
CO	3.85199	.09709	1.65096	0	2.20103
Hydrogen	7.50853	2.58543	0	7.50853	0
CO2	.25697	3.93122E-3	.07007	0	.18689
Acetylene	10.7246	.29112	9.89996	.82472	0
Ethylene	1.32871	3.34925E-2	1.13884	.18987	0
Ethane	2.25909E-4	5.31479E-6	1.80727E-4	4.51818E-5	0
Propylene	.08702	1.46244E-3	.07459	1.24361E-2	0
Benzene	2.45733	2.17528E-2	2.26836	.18896	0
Paraffins	.45394	3.81413E-3	.38907	.06486	0
Olefins	1.96814	1.56965E-2	1.60118	.26695	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	1.34835	3.66018E-2	0	.14980	1.19854
Other	0	99.1486	0	0	0
Gas Total:	39.2290	100	24.1761	11.5671	3.58647

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passes through the sample as shown in Fig. 5. Depending on the geometry of the sample stream, either focused or parallel optics were used as the beam passed through the sample. Figure 5 shows the arrangement for focus optics. The EFR uses focussed optics. Emission measurements are made with the movable mirror (see Fig. 5) in place. Transmission measurements are made with the movable mirror removed. The emission and transmission can be measured for the same sample volume. In an ideal emission-transmission experiment, both measurements would be made simultaneously. In our case the emission and transmission measurements are made sequentially in time along the same optical path, for a sample flowing in a nominally steady condition. The technique is rapid; a low noise emission or transmission spectrum at low resolution (4 cm^{-1}) can be recorded in under a second. Also, the radiation is amplitude modulated by the interferometer, and only such radiation is detected. Because of its unmodulated nature, the emission passing directly to the detector does not interfere with the measurements of transmission, provided saturation of the detector is avoided. Care must also be exercised to insure that emission from the sample incident on the interferometer is not scattered back to the transmission detector.

Theoretical Background

For multi-phase reacting systems, measurements are made of the transmittance and the radiance, and from these, a quantity called the normalized radiance is calculated. The analysis which follows Siegel and Howell (16) has been presented previously (17). The relevant equations for a homogeneous medium are presented below.

Transmittance. T_ν - The transmittance, T_ν, is defined in the usual manner,

$$T_\nu = I_\nu / I_{0\nu},\qquad(1)$$

where $I_{0\nu}$ is the intensity transmitted in the absence of a sample stream, while I_ν is that transmitted with the sample stream in place. For a medium containing gases and soot particles with absorption coefficients α_ν^g and α_ν^s, respectively, the transmittance can be expressed as

$$T_\nu = \exp\left(-(\alpha_\nu^s + \alpha_\nu^g)\, L\right)\qquad(2)$$

where L is the path length. T_ν is sometimes plotted as a percent.

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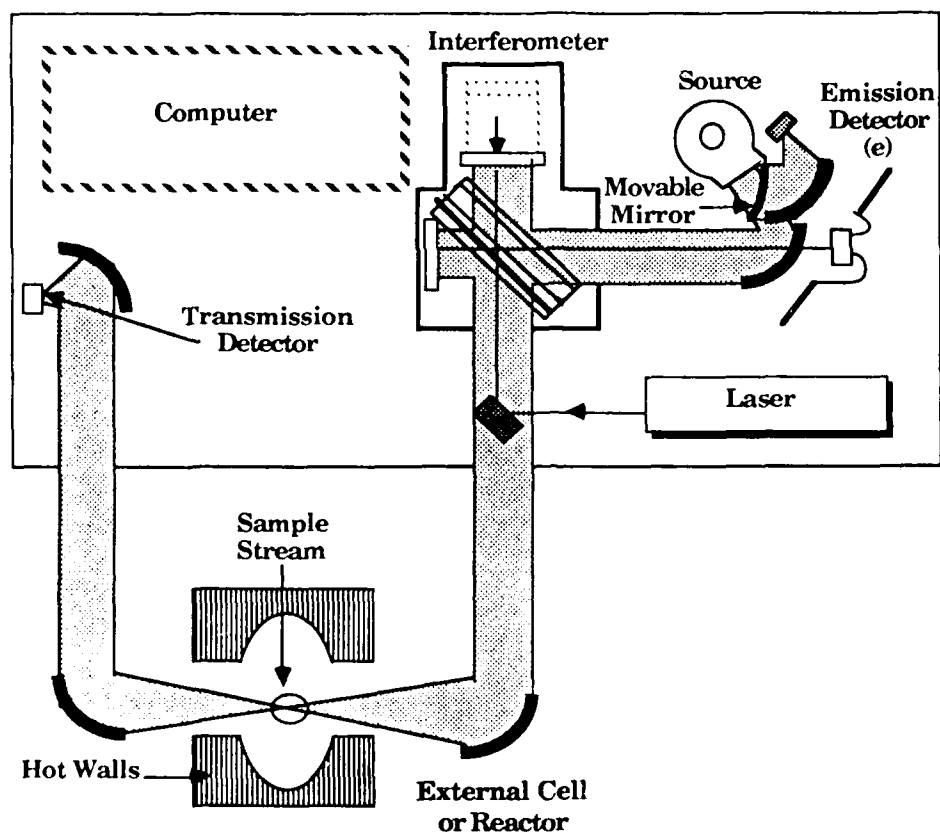
Figure 5. FT-IR Spectrometer with External Cell or Reactor.

Radiance, R_ν - To determine the sample radiance R_ν, the radiative power emitted and scattered by the sample is measured, and the background subtracted to obtain, S_ν. This is then converted to the sample radiance,

$$R_\nu = S_\nu / W_\nu \tag{3}$$

where W_ν is the instrument response function measured using a black-body cavity. We can also express R_ν in terms of properties of the constituent phases of the sample, where it is given by (16,17)

$$R_\nu = \frac{\left[\alpha_\nu^s R_\nu^b(T_s) + \alpha_\nu^g R_\nu^b(T_g)\right] \cdot \left[1 - \exp(-(\alpha_\nu^s + \alpha_\nu^g)L)\right]}{\alpha_\nu^s + \alpha_\nu^g} \tag{4}$$

where $R_\nu^b(T_g)$ and $R_\nu^b(T_s)$ are the Planck black-body functions at the temperatures of the gas and soot, respectively. In deriving this expression we have assumed no scattering for soot particles in the IR region.

Normalized Radiance, R_ν^n - The normalized radiance, R_ν^n, is defined as

$$R_\nu^n = R_\nu / (1 - \mathcal{T}_\nu). \tag{5}$$

From Eqs. (2) and (4), the normalized radiance is

$$R_\nu^n = \frac{\alpha_\nu^s R_\nu^b(T_s) + \alpha_\nu^g R_\nu^b(T_g)}{\alpha_\nu^s + \alpha_\nu^g} \tag{6}$$

Soot Under Pyrolysis Conditions - This section considers the case of mixtures of soot particles and gases. In the simplest case, soot particles were formed by the pyrolysis of butane in nitrogen in the entrained flow reactor at 1573 K. For one case, the butane was confined to the center of the reactor, for the second, it was dispersed more uniformly across the reactor. Figure 6 shows $\mathcal{T}_\nu$, R_ν and R_ν^n for the first case. The transmittance spectrum shows a sloping continuum, typical of soot particles, with the absorption bands for gases, mainly CO_2, acetylene, methane, ethylene and PAH's, superimposed on the continuum. From Eq. (2) $\mathcal{T}_\nu = \exp(-(\alpha_\nu^s + \alpha_\nu^g)L)$, where α_ν^s is proportional to the volume fraction of soot particles.

- 15 -
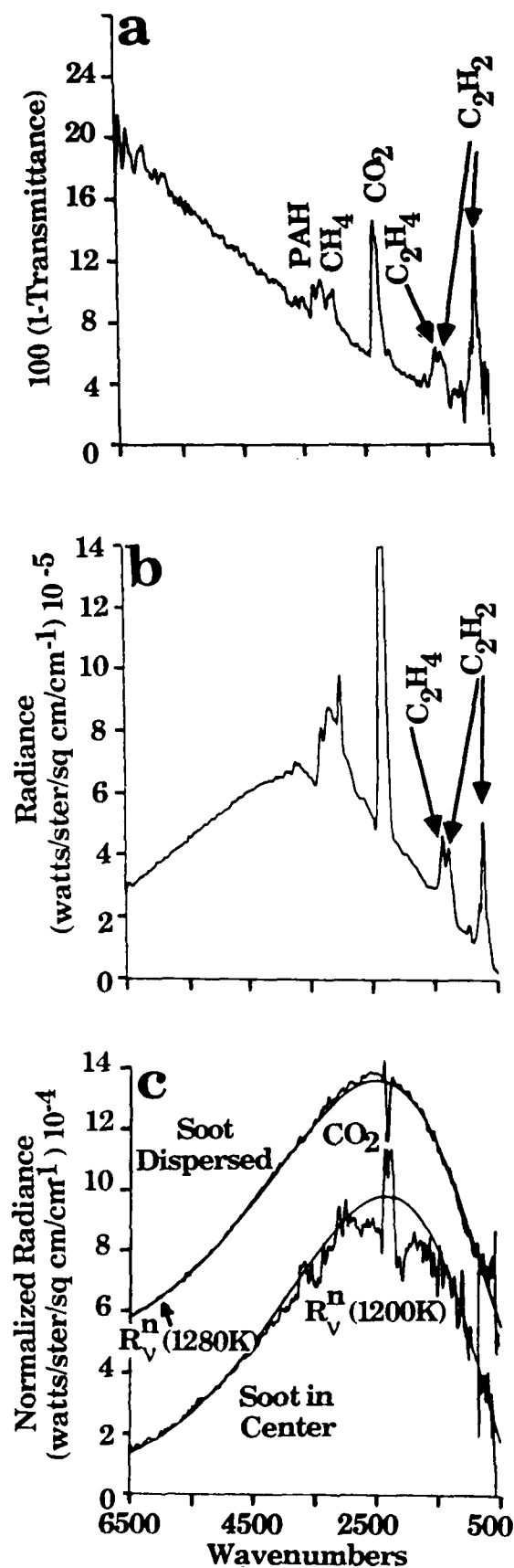
Figure 6. Butane + CO_2 Pyrolyzed in Nitrogen in the Entrained Flow Reactor at 1573 K with 66 cm Reaction Distance. a) 100(1-Transmittance), b) Radiance and c) Normalized Radiance. Upper Curves in c (displaced vertically for clarity) is for Dispersed Soot). All other Curves are for Soot at Center of Reactor.

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The soot temperature is determined from the measured spectrum, R_ν^n, Fig. 6c (lower curve). In regions where α_ν^g is zero, $R_\nu^n = R_\nu^b(T_s)$. A theoretical black body curve for $T_s = 1200$ K yields the best match to the experimental curve in both spectral shape and amplitude in the regions away from the gas bands. The uncertainty in determining R_ν^n is typically within $\pm 5\%$. At 1200 K this results in ± 30 K uncertainty in temperature.

Both shape and amplitude will fit precisely only if there is no variation in temperature over the optical path. If such a variation exists, the spectral shape can be matched with that of a theoretical black body curve, but at some fraction of the theoretical amplitude. Fitting the shape alone will give an average temperature. We have therefore fit the shape alone in a separate determination for a temperature of 1230 K. In this case, the two approaches agree to within 30 K.

According to Eq. (6), if T_g and T_s were equal, R_ν^n would equal R_ν^b over the whole spectrum. This is not the case, most clearly for the CO_2 which appears to be at a higher temperature than the soot. To obtain the gas temperature once T_s is known, Eq. (6) can be rearranged to give,

$$R_\nu^b(T_g) = R_\nu^n + (R_\nu^n - R_\nu^b(T_s))(\alpha_\nu^s/\alpha_\nu^g) \tag{7}$$

Since the right hand side of Eq. (7) is known, T_g can be obtained. The gas temperature is determined to be 1300 K from the CO_2 band at 2300 cm^{-1}, in good agreement with the suction pyrometer measurement of 1295 K. The difference between the soot and gas temperatures is believed to be due to the radial distribution of soot and CO_2 in the reactor. The soot, which is concentrated along the center line of the reactor is 70 K lower than the average gas temperature. To confirm this hypothesis, a second experiment was performed in which the butane was dispersed throughout the reactor tube. The results are shown in Fig. 6c (upper curve) which has been displaced vertically. The average soot and CO_2 temperature is 1280 K, in much better agreement with the suction pyrometer (1295 K). The narrow dip observed in the spectrum is an artifact due to room temperature CO_2 in the optical paths.

Measurements

For spectral regions away from the gas lines so that $\alpha_\nu^g = 0$ Eq. (2) becomes

$$\tau_\nu = \exp(-\alpha_\nu^s L) \tag{2a}$$

and Eq. (4) becomes $R_W^b(T_s)*(1-\mathcal{T}_\nu)$. Thus the radiance spectrum is very simply related to the transmission spectrum, and either one can be used as a measure of α_ν^S. With the assumption that the extinction coefficient $\alpha_\nu^S L$ is small, we can expand Eq. (2a) to

$$\mathcal{T}_\nu = 1 - \alpha_\nu^S L$$

or

$$\alpha_\nu^S L = 1 - \mathcal{T}_\nu \tag{2b}$$

This is typically done on our analyses.

The assumption that the scattering is small (used in deriving Eq. (2)) implies that we are in the Rayleigh limit where extinction coefficient, α_ν^S is proportional to the volume fraction of the particle times $1/\lambda$. The "constant" of proportionality depends on the optical constants of the soot. For the wavelength region we use in our spectroscopy (1.5μm to 20μm), we should be in the small particle regime for particles less than 0.3μm, which should be characterized by a straight plot of $1-\mathcal{T}_\nu$ vs $1/\lambda$. For particles at the high end of this size range, the optical constants will be independent of particle size, and we can compute a soot volume fraction from $(1-\mathcal{T}_\nu)$ and a knowledge of the optical constants. For very small particles, the optical constants may not be constant. This could be the case for very young soot (a few hundred angstroms in diameter) or PAH's, where the optical properties are just developing. This could result in $1-\mathcal{T}_\nu$ spectra which are not linear in $1/\lambda$. The relatively straight line in Fig. 6a is typical of the data we see for all of the fuels.

The procedure for obtaining emission/transmission data (1) is similar to that for the mass balance runs except that the products were usually not collected. To determine the soot concentrations (and temperatures) from the E/T experiments, the following experimental procedure was used: 1) Background transmission scans (I_0 in Eq. (1)) are taken before and after the sample transmission scan (I_ν in Eq. (1)). These background scans are averaged in the computation of the transmittance. 2) The mirror (Fig. 5) is switched to emission mode and a background emission spectrum is taken to measure background gases in the furnace (Fig. 7a) followed by the measurement of the emission with the fuel flowing (Fig. 7b). The background emission is subtracted from the sample emission, and the difference divided by the instrument response function (Fig. 7c) to obtain the sample radiance (Fig. 7d and Eq. (3)). The instrument response function was measured using a hot oxidized rod in the reactor as a reference black-body. 3) Finally, the 1-T curve is divided by

- 18 -
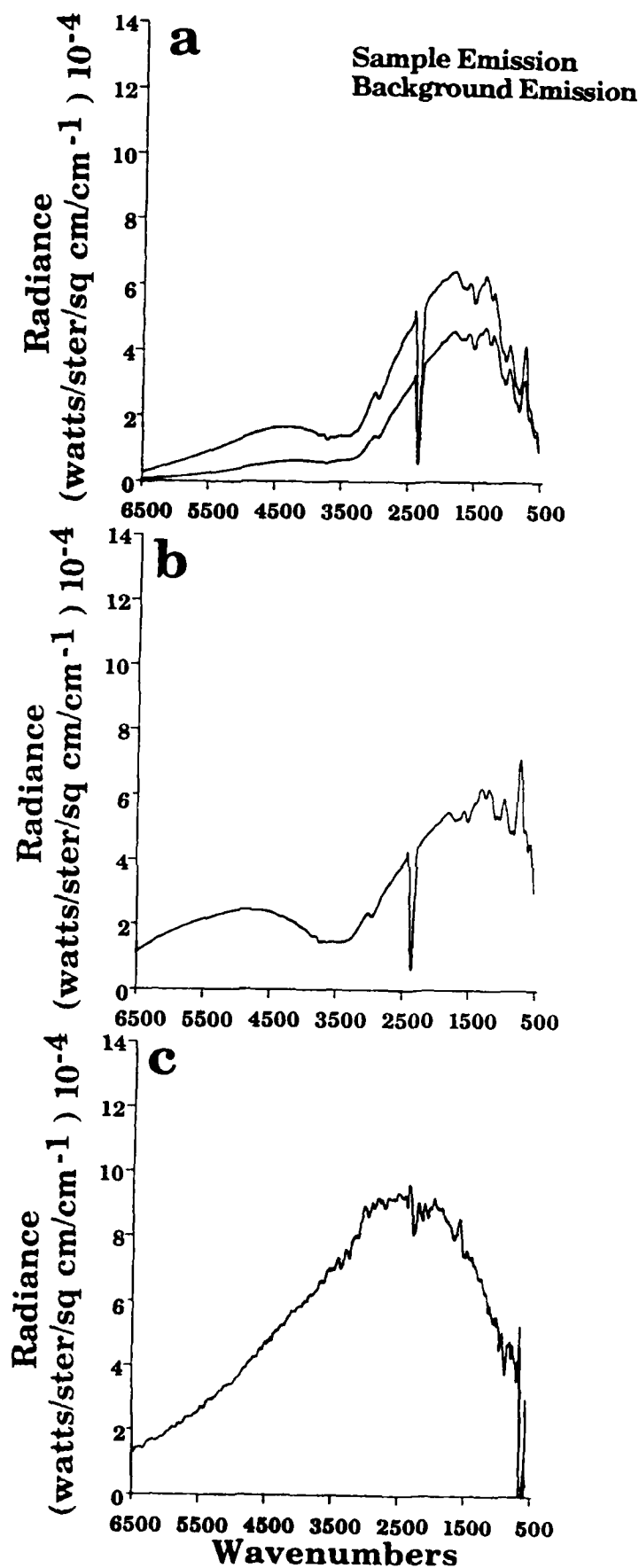
Figure 7. Sample Radiance Computation. a) Background and Sample Emission, b) Instrument Response Function for Black-Body Emitter and c) Sample Radiance.

the sample radiance (Eq. (5)) to obtain the normalized radiance. For the purpose of the experiments reported here, the normalized radiance (which should be a black-body curve at the temperatures of the soot (Eq. (7)) was used as a consistency check on the radiance and transmission data.

Heated Tube Reactor (HTR)

The heated tube reactor is illustrated in Fig. 8. It consists of a 5.08 mm ID Inconel 702 tube which is heated electrically. Fuel, entrained in cold carrier gas, is injected at the top of the tube. The fuel-gas mixture enters the heated section of the tube and heats rapidly. The heat transfer rate is large because of the small tube diameter, the high thermal conductivity and low heat capacity of the helium carrier gas, and the fact that the particles collide with the hot walls of the tube. After a variable residence time, the reacting stream is either ejected from the tube end for temperature and velocity measurements, or is quenched in a water cooled section of the tube for mass balance measurements. The product collection train is the same as for the EFR. The heated tube reactor can be used at temperatures up to 800°C and 20 atmospheres, and was used for the pressure experiments in Task V.

High Pressure Reactor (HPR)

To study the variation of pyrolysis behavior of hydrocarbons with pressure, a high pressure version of the EFR was made available to this program. Maximum specifications are: temperatures up to 1650°C, pressures up to 600 psig, 5 second residence times and 0.6 lbs/hr fuel throughput. We used this reactor for this program, but the initial results on 6 fuels were not useful.

The reactor design is illustrated in Fig. 9. The furnace consists of a high pressure shell (capable of containing pressures up to 600 psig), a thick layer of insulation and a high temperature region heated by Kanthal Super 33 electrical heating elements. The high temperature section (capable of temperatures up to 1650°C) contains an alumina bed heat exchanger and a test section. The ambient gas enters the furnace through the heat exchanger to bring it up to furnace temperature and then turns downward into the test section. Fuel is injected at a fixed point at the top of the test section using a water cooled injector. It mixes with the ambient gas and, after a fixed distance, enters a water-cooled collector. The reaction products then enter a cyclone to separate char, followed by a filter to remove tar and soot. The gas stream is reduced in pressure and collected in a
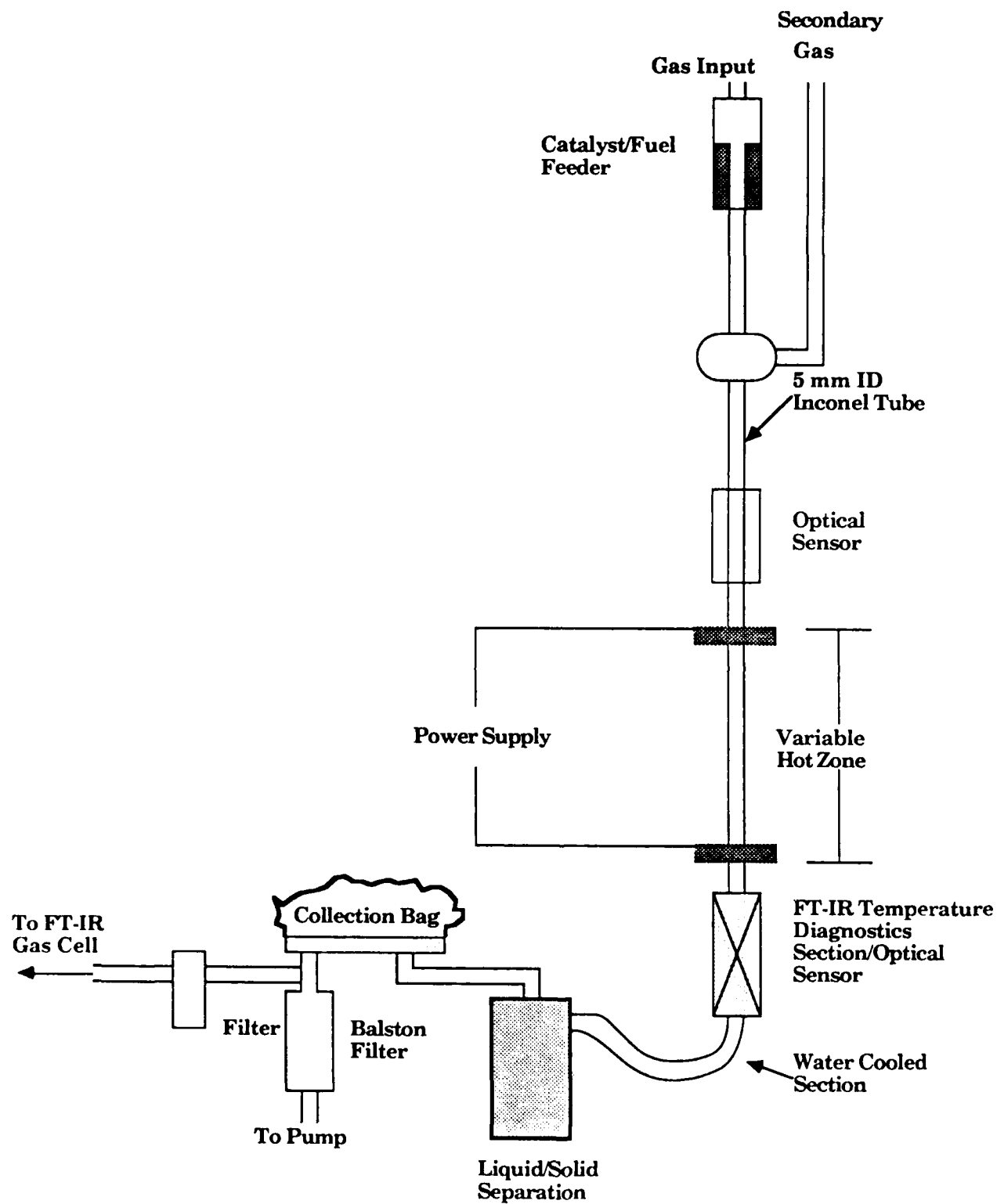
Figure 8. Schematic of Heated Tube Reactor.
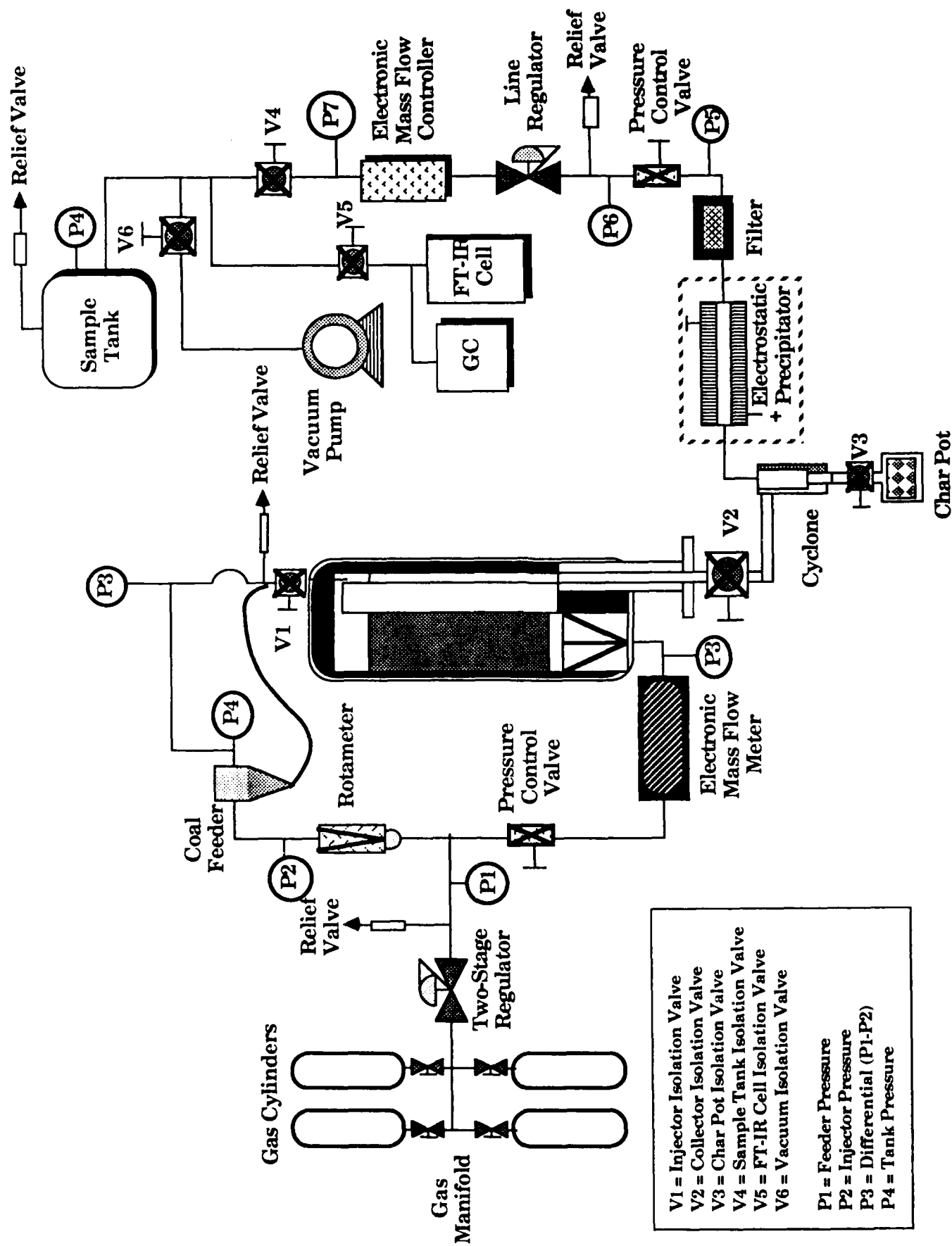
Figure 9. Schematic of High Pressure Entrained Flow Reactor System.

V1 = Injector Isolation Valve
V2 = Collector Isolation Valve
V3 = Char Pot Isolation Valve
V4 = Sample Tank Isolation Valve
V5 = FT-IR Cell Isolation Valve
V6 = Vacuum Isolation Valve

P1 = Feeder Pressure
P2 = Injector Pressure
P3 = Differential (P1-P2)
P4 = Tank Pressure

holding tank. The tank is a steel tank with glass-lined walls which is used to collect the total gaseous effluent from the reactor system during a typical run. It is initially evacuated and, during a run, the pressure gradually increases as it fills. After an experiment, a sample is taken from the tank and analyzed in an FT-IR cell and a GC.

The gas supply to the reactor is from a bank of high pressure cylinders connected by a manifold. The high pressure in the cylinders (2500 psi) is reduced down to the working pressures (10-200 psi) via a two-stage regulator. The gas supply is split into a carrier stream for the feed system and a main gas stream for the reactor. An electronic mass flow meter (MFM) is used to monitor the main gas flow into the reactor system. An electronic mass flow controller (MFC) downstream of the reactor is used to maintain a constant mass flow of gas through the system under stable reactor conditions.

For the liquid fuels in this program, no useful results were obtained. In several test experiments in the HPR, the mass balance was poor, presumably due to loss of soot, tar, and liquid fuel (condensibles) in the cooler outer shell of the HPR. Even with butane there was too much missing mass. As a result the only pressure results are those obtained in the HTR.

TGA/FTIR

The thermogravimetric analyzer/FTIR (TGA/FTIR), illustrated in Fig. 10, consists of a sample suspended from a balance in a programmable furnace (18). The evolved products are swept into a gas cell for analysis by FT-IR. The FT-IR allows on-line measurements of the gas and tar concentration and composition. On this program, the TGA/FTIR was used only to determine the tar/soot balance of the solids collected from the EFR.

Droplet Generator

In the initial contract, the fuels were to be fed as a steady stream of regularly spread droplets. Although this was changed in the contract redirection a version of a feeder based on one described by Maloney, et al. (19) was constructed and successfully tested. It consisted of a cylindrical piezoelectric tube (4 mm ID, 6 mm OD and 5 cm long) fed by a reservoir of fuel from one end, and with a hypo tube ejector tip on the other. The crystal was driven by a specially constructed high voltage pulse generator, whose pulse duration and repetition rate could be adjusted. It produced a steady stream of regularly spaced single-sized droplets in bench tests.
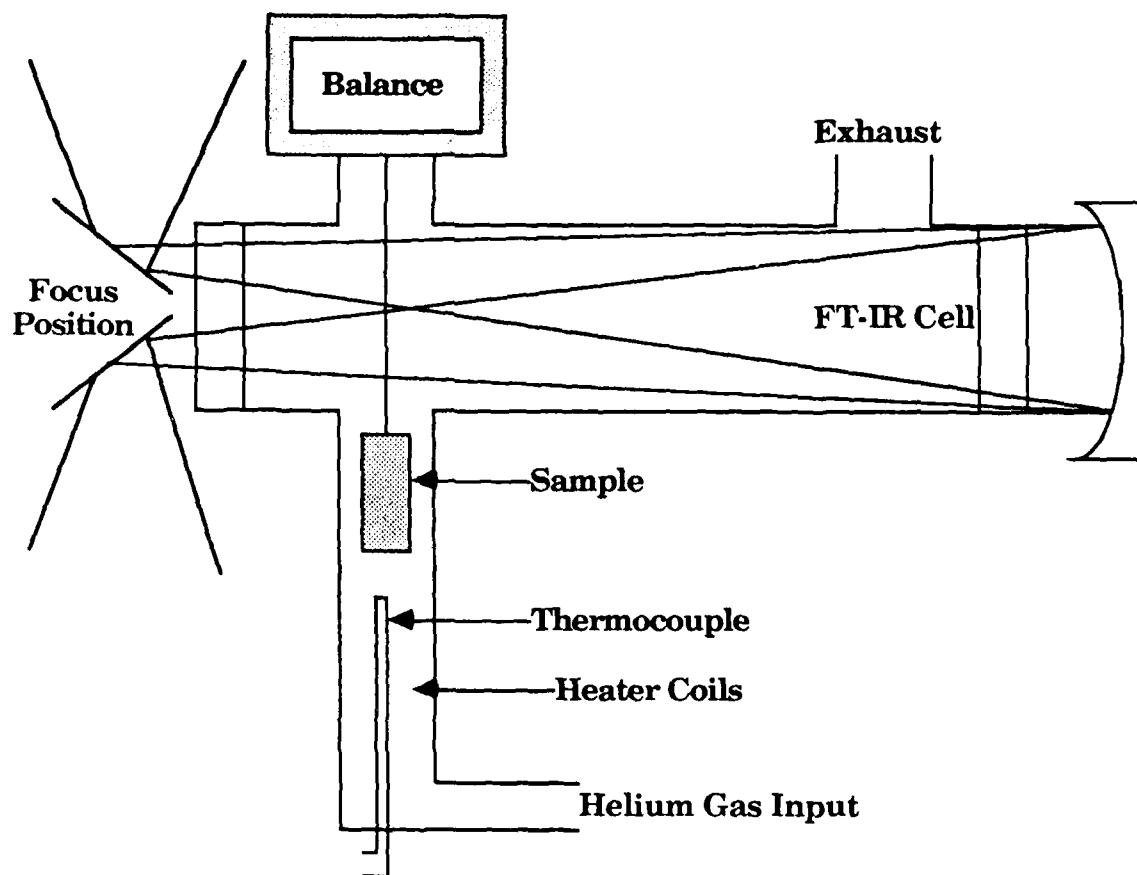
Figure 10. EGA/TGA Block Diagram.

III. RESULTS

TASK I - Mechanistic Studies of Pyrolysis, Combustion, and Soot Production.

In this task, data were obtained on 31 hydrocarbon fuels. In addition, six pure hydrocarbons, acetylene, benzene, butane, decalin, tetralin and dodecane were analyzed. The measurements performed are summarized in Table 2.

The fuels analyzed were the 25 fuels from the NASA study (20) provided by the Air Force, plus the four JP8X's, also provided by the Air Force. The 25 fuels from NASA were selected and blended by NASA and UTRC to provide a range of naphthalene, hydrogen and total aromatic content. The naphthalene ranged from 0 to 29.7 wt.%; the hydrogen from 9.1 to 15.0 wt.%, and total aromatics from 0 to 100 %. The soot production as indicated by EFR data ranged from 28 to 68 wt.%. The JP8X's were blended to provide a range of aromatic contents (20%-45%).

The pyrolysis results are summarized in Figs. 11 through 26 for the major products, and the full product slates are shown in Appendix A, Tables A-1 through A-109.

The measurements consist of three classes: 1) mass balance experiments, where all the products are measured, 2) E/T experiments, for which a correlation with soot quantity was sought, and 3) liquid cell spectra which were used in the correlation studies of Task II.

Mass Balance Data

As indicated in Table 2, all of the fuels were pyrolyzed at 1300°C with the injector set at 66 cm (about 700 ms residence time) using the EFR with the heated injector. These conditions were chosen as a standard base condition which provided partial conversion to soot, and should provide a good relative measure of the sooting potential of the fuels.

For several of the fuels (tetralin, decalin, butane, acetylene, benzene, dodecane, and the 4 JP8X's) profiles were obtained as a function of injector position at (i.e. residence time) 1300°C. The major species are shown in Figs. 11 through 26. In addition, full butane series were measured at 1300°C with added 3.0 vol% H_2 or O_2 (Figs. 20 and 21), and at 66 cm as a function of temperature (Fig. 19). The butane and acetylene series were measured at 1100°C (Figs. 17 and 23) and the acetylene at 1500°C (Fig. 24).

TABLE 2

SUMMARY OF FUELS AND EXPERIMENTS

FUELS	EFR Pyrolysis	In-Situ Scan	E/T Data
UTRC 2A	1300°C, 66 cm		1400°C, 66 cm 1300°C, 66 cm 1100°C, 66 cm
ERBLS 1	1300°C, 66 cm		1300°C, 66 cm
UTRC 7A	1300°C, 66 cm		
JP7	1300°C, 66 cm		1300°C, 66 cm
JP4-S	1300°C, 66 cm		
JP4	1300°C, 66 cm		1300°C, 66 cm
DF2	1300°C, 66 cm		1300°C, 66 cm ($+H_2$, $+O_2$) 1400°C, 66 cm ($+H_2$)
AFAPL 6	1300°C, 66 cm		1300°C, 66 cm ($+H_2$, $+O_2$)
AFAPL 2	1300°C, 66 cm		1300°C, 66 cm
UTRC 3B	1300°C, 66 cm		
UTRC 8A	1300°C, 66 cm		
ERBLS 2	1300°C, 66 cm		1300°C, 66 cm ($+H_2$)
UTRC 9A	1300°C, 66 cm		1300°C, 66 cm
UTRC 9B	1300°C, 66 cm		
Tetralin	1300°C, 24, 46, 56, 66 cm	yes	
XTB	1300°C, 66 cm		1400°C, 66 cm ($+H_2$, $+O_2$) 1300°C, 66 cm 1100°C, 66 cm
BLS	1300°C, 66 cm		1300°C, 66 cm ($+H_2$, $+O_2$)

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TABLE 2 (continued)

ERBLS 3	1300°C, 66 cm		
ERBS	1300°C, 66 cm		
Decalin	1300°C, 26, 46, 56, 66 cm	yes	1400°C, 66 cm ($+H_2$, $+O_2$) 1300°C, 66 cm
JP4-A	1300°C, 66 cm		
Jet A	1300°C, 66 cm		1300°C, 66 cm ($+H_2$, $+O_2$)
JP5	1300°C, 66 cm		1300°C, 66 cm ($+H_2$, $+O_2$)
GMSO	1300°C, 66 cm		
UTRC 1	1300°C, 66 cm		
JP8X-2414 (45% aromatic)	1300°C, 26, 46, 56, 66 cm	yes	1400°C, 66 cm 1300°C, 66 cm
JP8X-2383 (20% aromatic)	1300°C, 26, 46, 56, 66 cm	yes	1300°C, 66 cm ($+H_2$, $+O_2$)
JP8X-2398 (30% aromatic)	1300°C, 26, 46, 56, 66 cm	yes	1300°C, 66 cm
JP8X-2429 (30% aromatic)	1300°C, 26, 46, 56, 66 cm	yes	1300°C, 66 cm
Butane	1100°C all 7 positions,	yes	
	1300°C all 7 positions, 1200, 1400, 1500°C, 66 cm	yes	
Butane + H_2	1300°C all 7 positions	yes	
Butane + O_2	1300°C all 7 positions	yes	
Acetylene	1300°C all 7 positions,		1300°C 8 positions
	1500°C all 7 positions*	yes	
	1100°C all 7 positions*	yes (shows no soot)	

TABLE 2 (concluded)

Benzene	1300°C all 7 positions	
Dodecane	1300°C, 24, 46, 56, 66 cm	yes

* contaminated with stabilizer

Note: 7 standard positions are 6, 16, 26, 36, 46, 56, and 66 cm
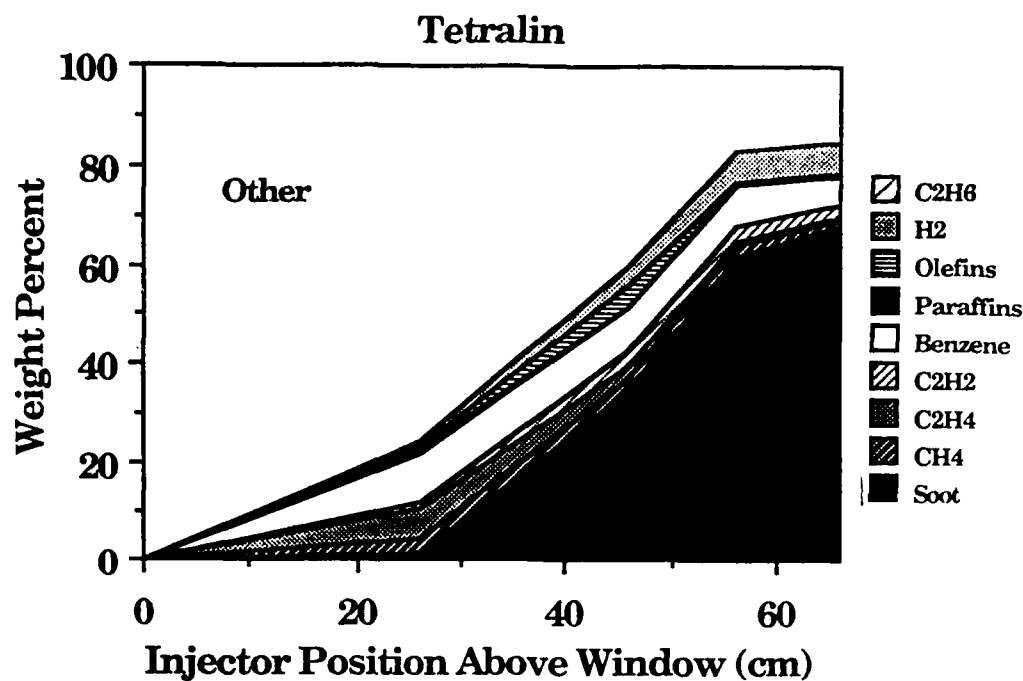
Figure 11. Pyrolysis Data for Tetralin as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm. "Other" Includes Raw Fuel.
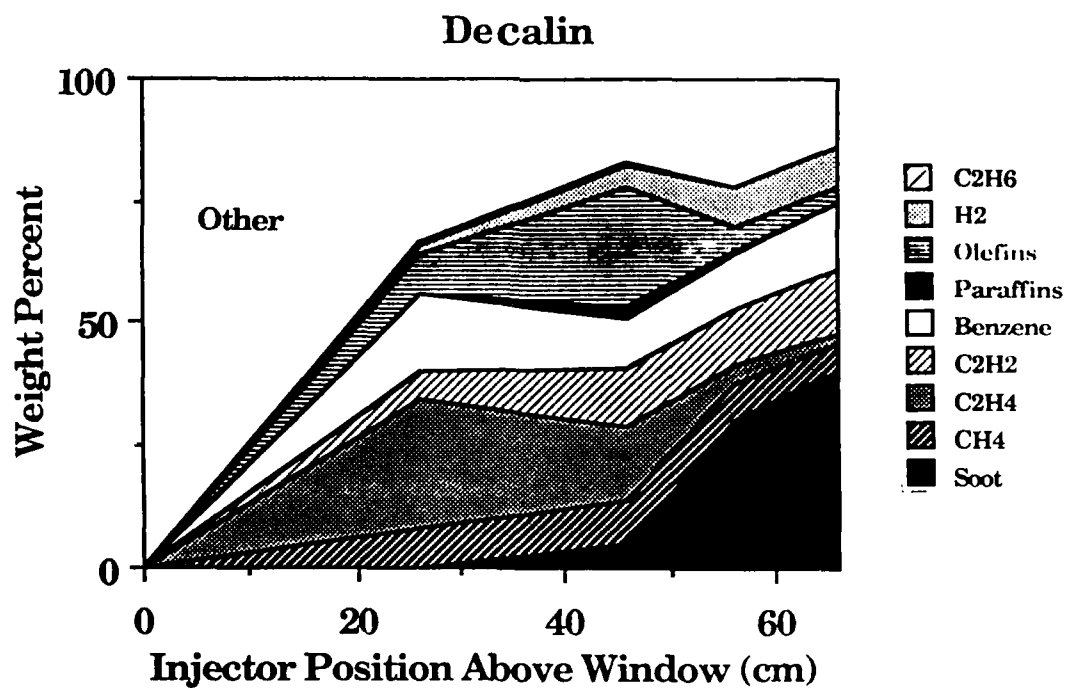
Figure 12. Pyrolysis Data for Decalin as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm. "Other" Includes Raw Fuel.

JP8X-2414 (45% ar)
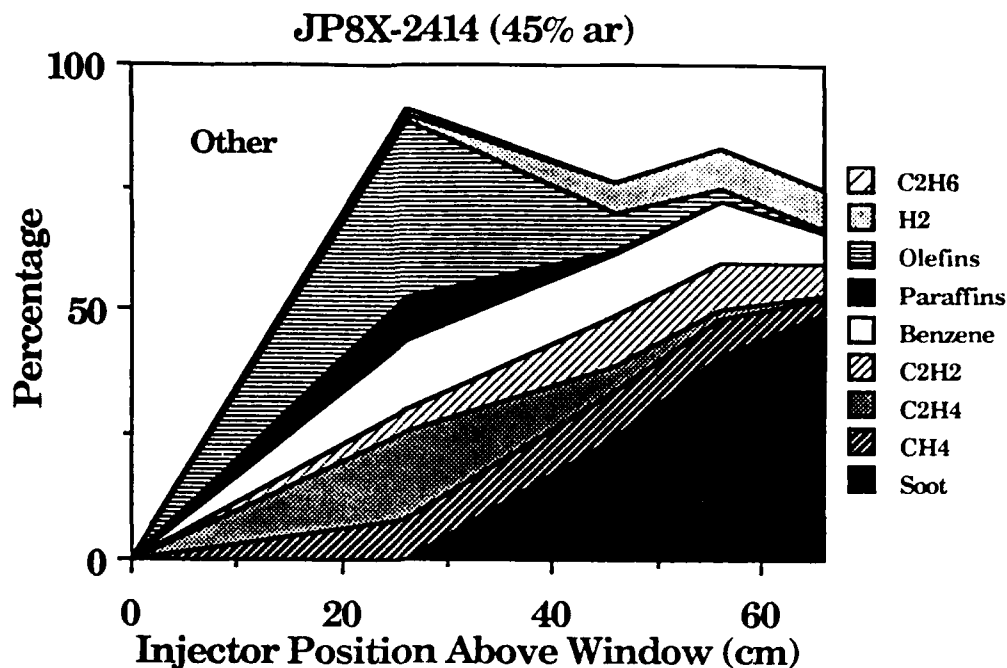
Figure 13. Pyrolysis Data for JP8X-2414 as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm. "Other" Includes Raw Fuel.

JP8X-2383 (20% ar)
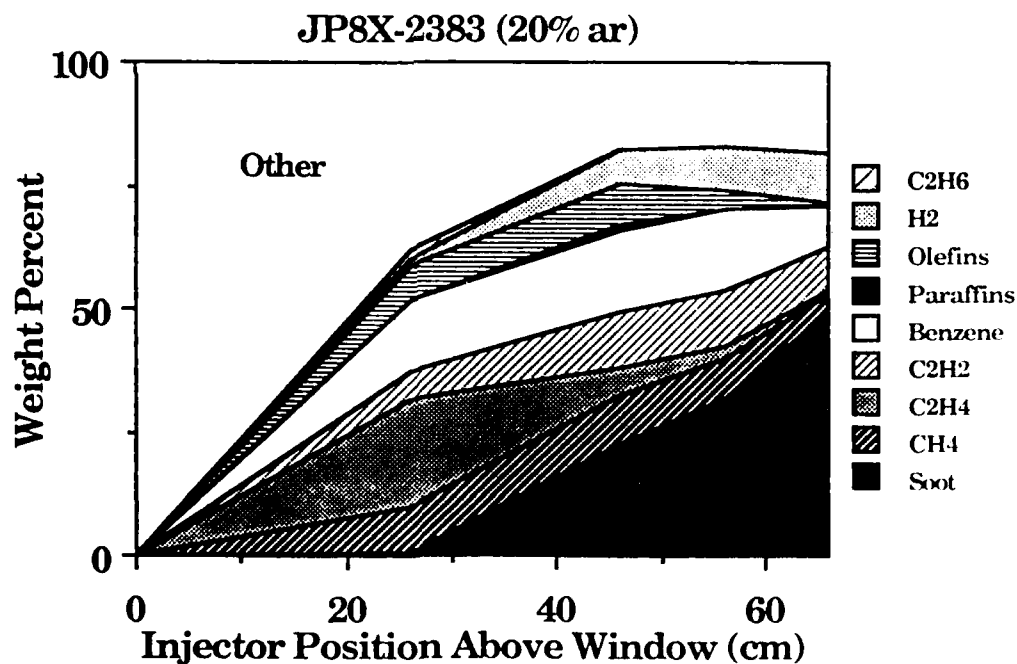
Figure 14. Pyrolysis Data for JP8X-2383 as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm. "Other" Includes Raw Fuel.
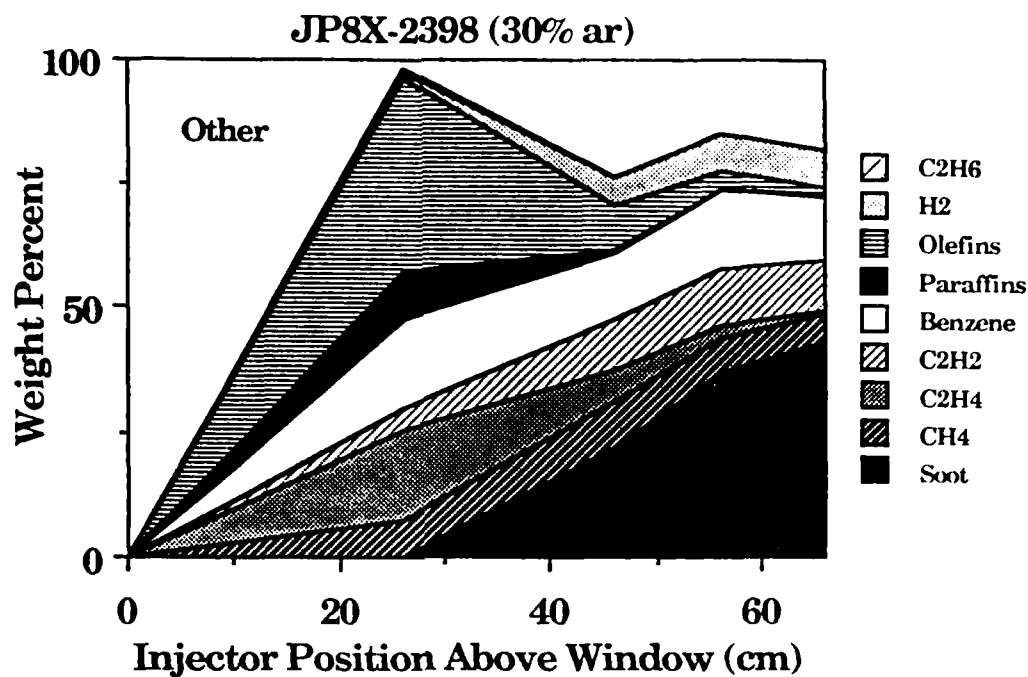
Figure 15. Pyrolysis Data for JP8X-2398 as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm. "Other" Includes Raw Fuel.
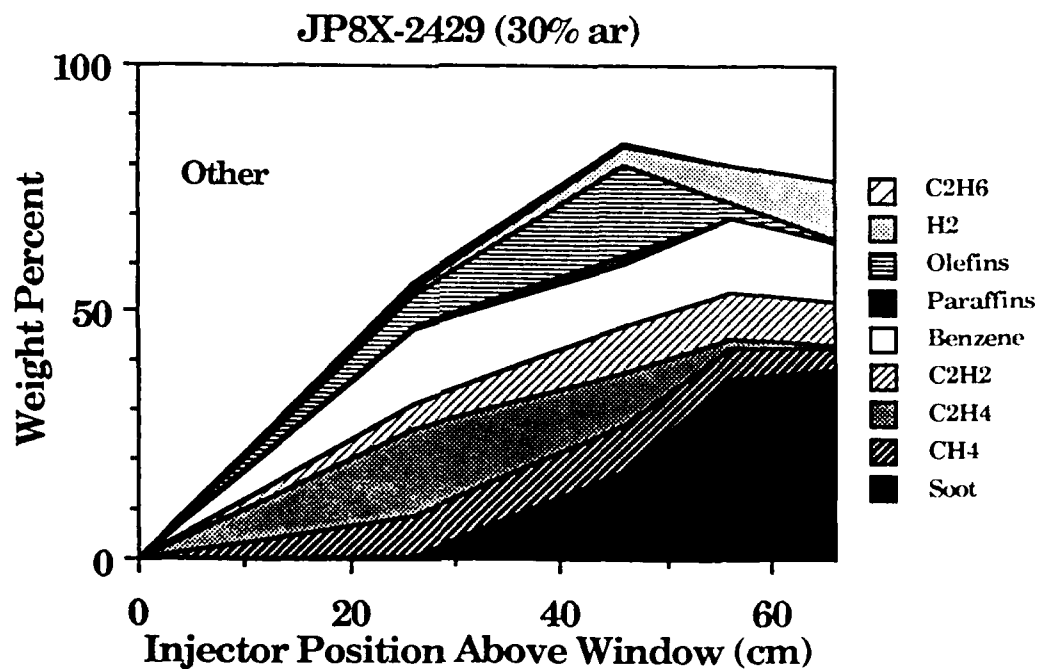
Figure 16. Pyrolysis Data for JP8X-2429 as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm. "Other" Includes Raw Fuel.

Butane Pyrolysis Data (1100°)
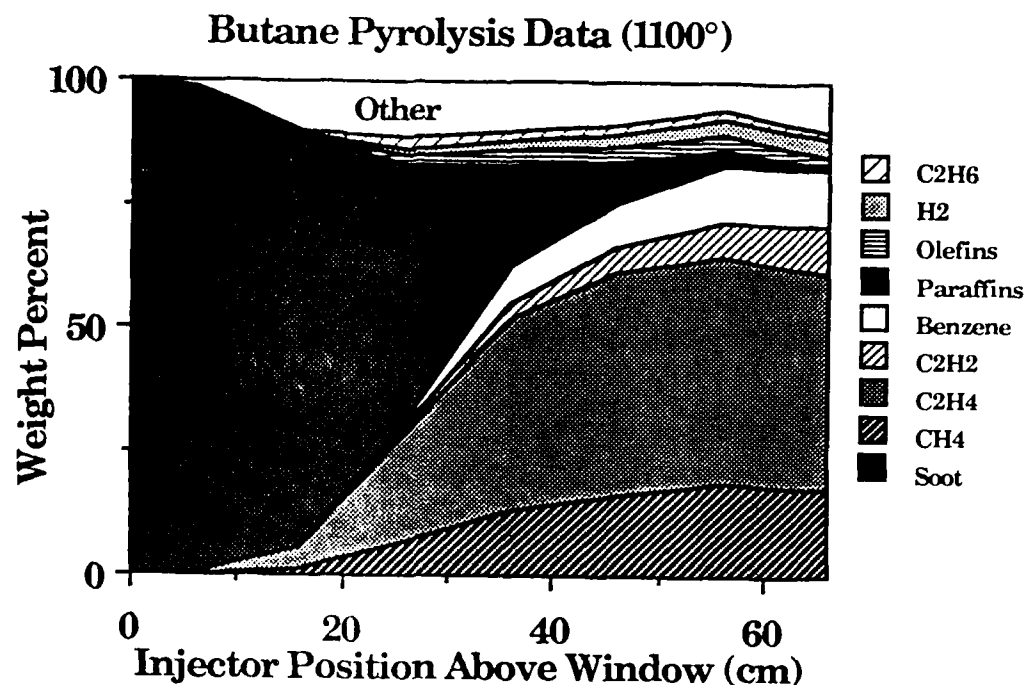
Figure 17. Pyrolysis Data for Butane as a Function of Injector Position at 1100°C. The Residence Time is Approximately 10 ms per cm.

Butane Pyrolysis Data (1300°)
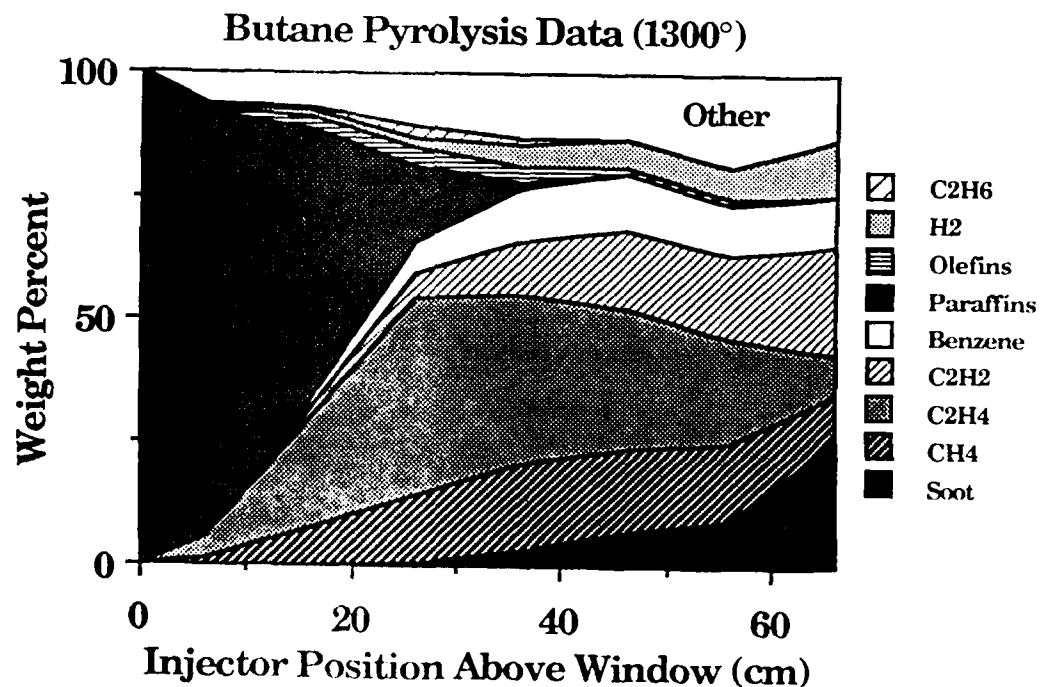
Figure 18. Pyrolysis Data for Butane as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm.

Butane vs Temperature
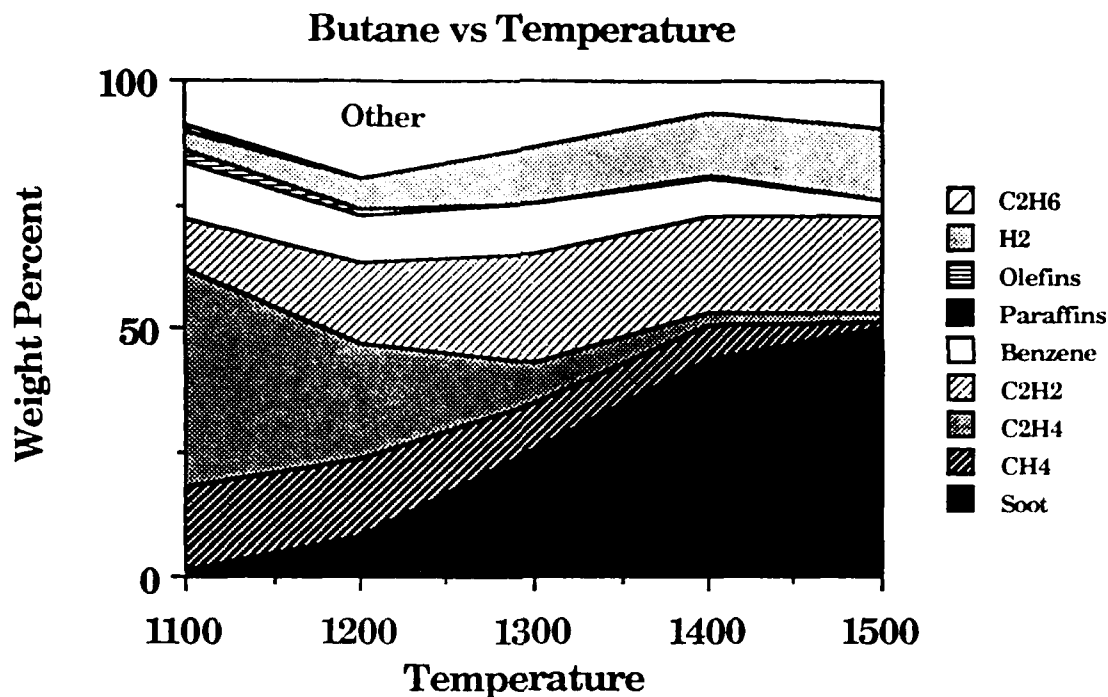
Figure 19. Pyrolysis Data for Butane as a Function of Temperature for an Injector Position of 66 cm. The Residence Time is Approximately 700 m s.

Butane Plus H2 1300°C
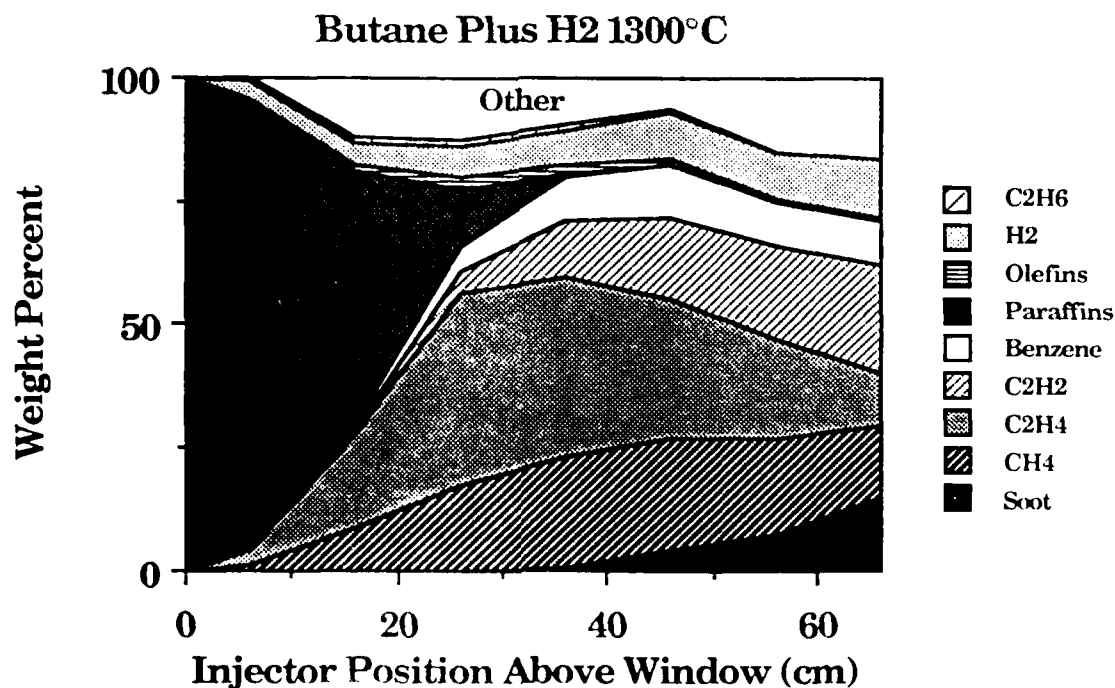
Figure 20. Pyrolysis Data for Butane + H2 as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 m s per cm.

Butane Plus O2 1300°C
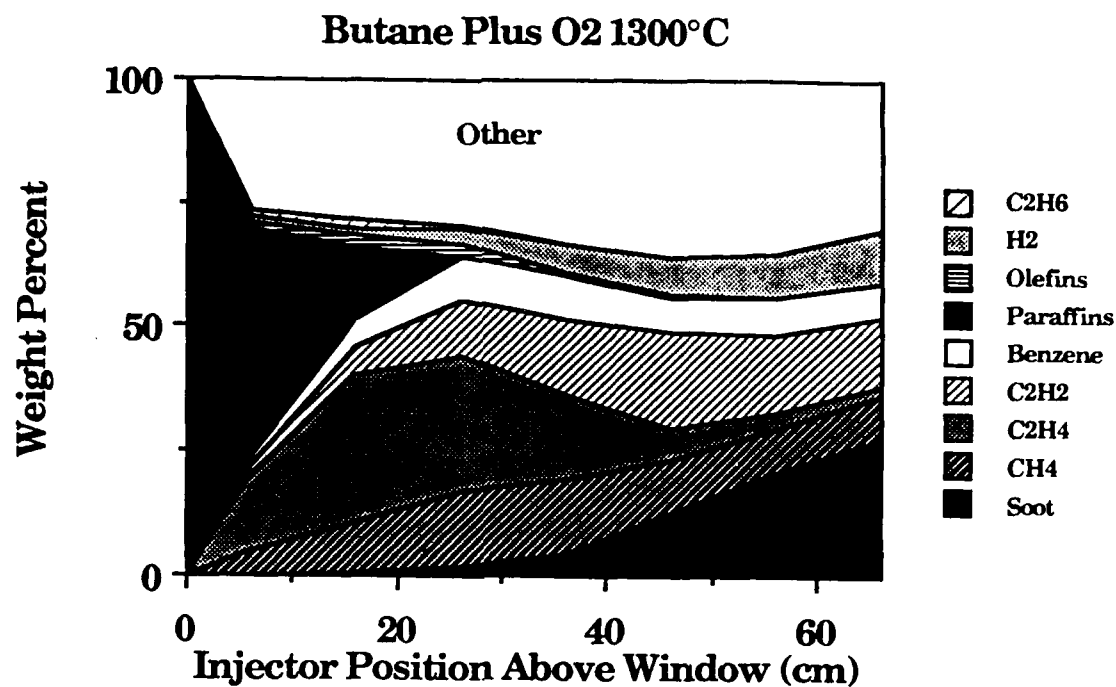
Figure 21. Pyrolysis Data for Butane + O_2 as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm.

Acetylene 1300° clean
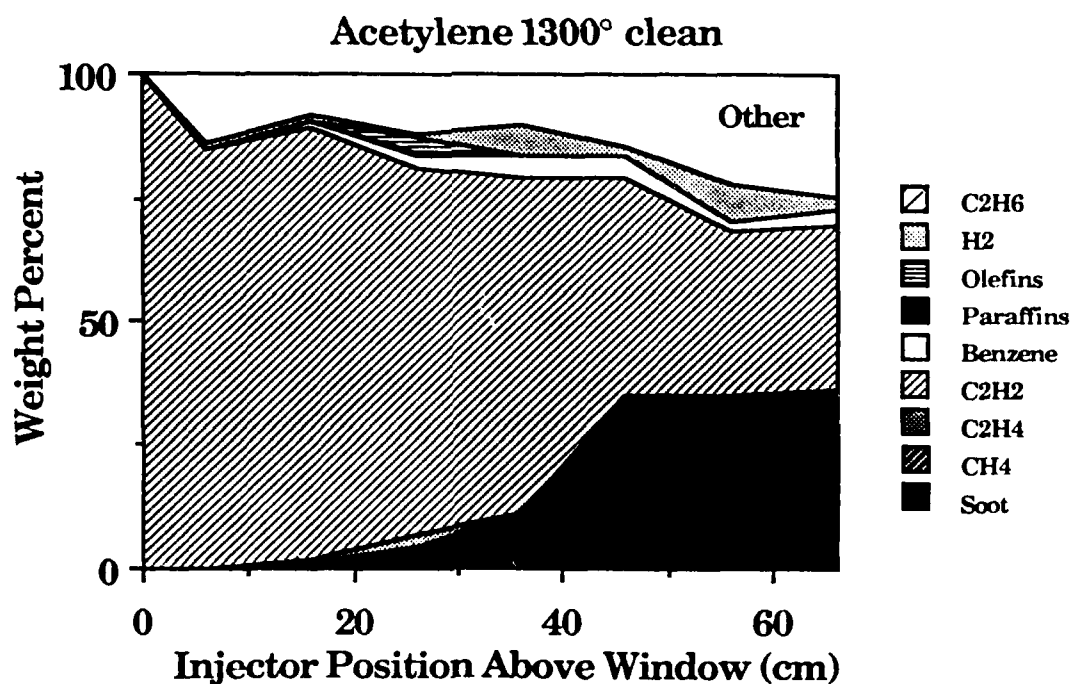
Figure 22. Pyrolysis Data for Acetylene as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm.
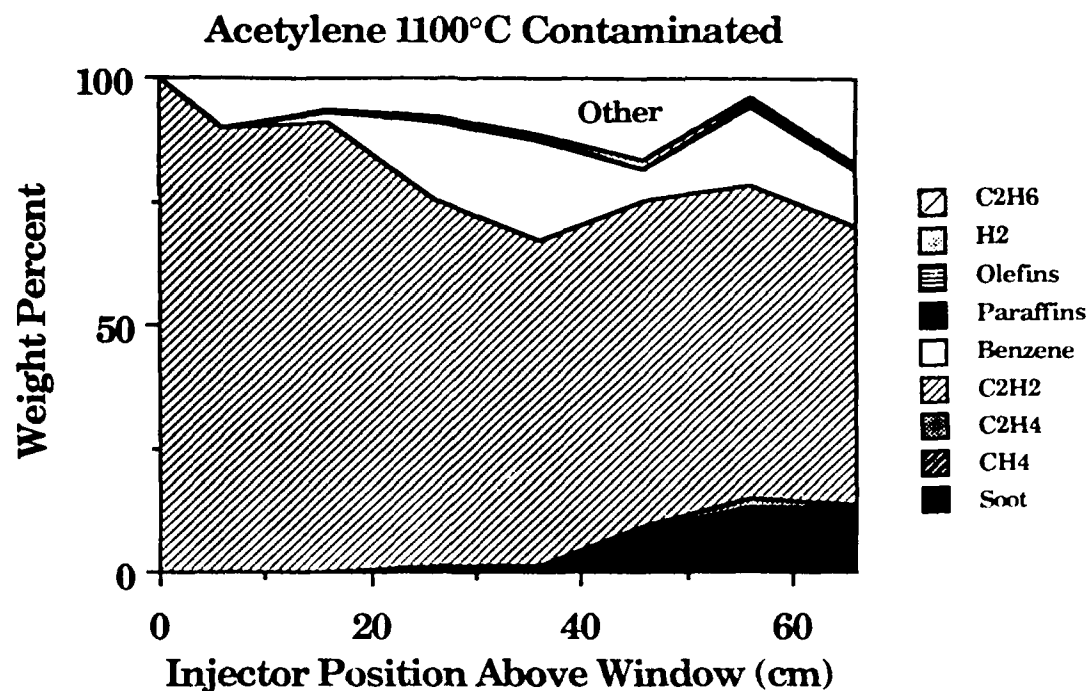
Figure 23. Pyrolysis Data for Acetylene as a Function of Injector Position at 1100°C. The Residence Time is Approximately 10 ms per cm.
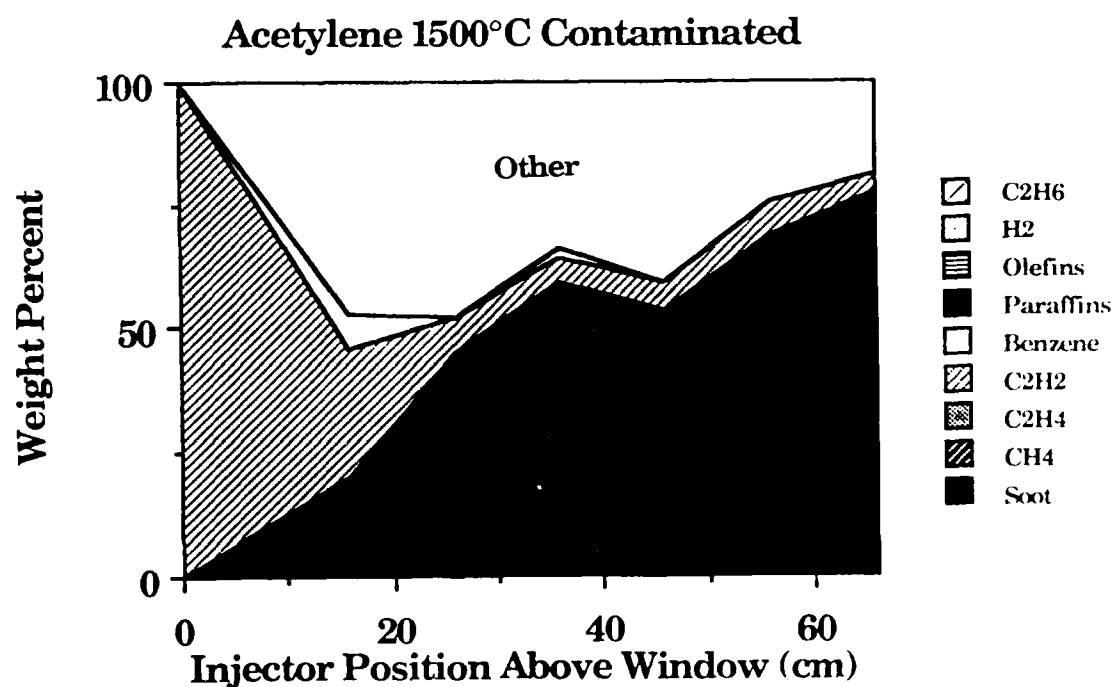
Figure 24. Pyrolysis Data for Acetylene as a Function of Injector Position at 1500°C. The Residence Time is Approximately 10 ms per cm.
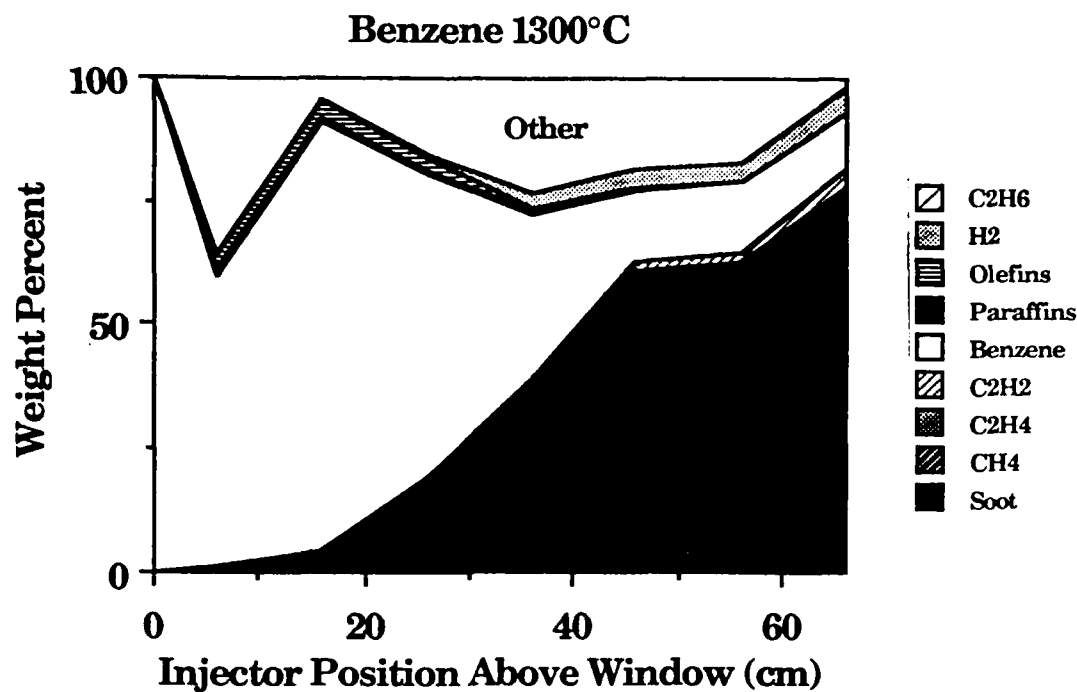
Benzene 1300°C

Figure 25. Pyrolysis Data for Benzene as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm.
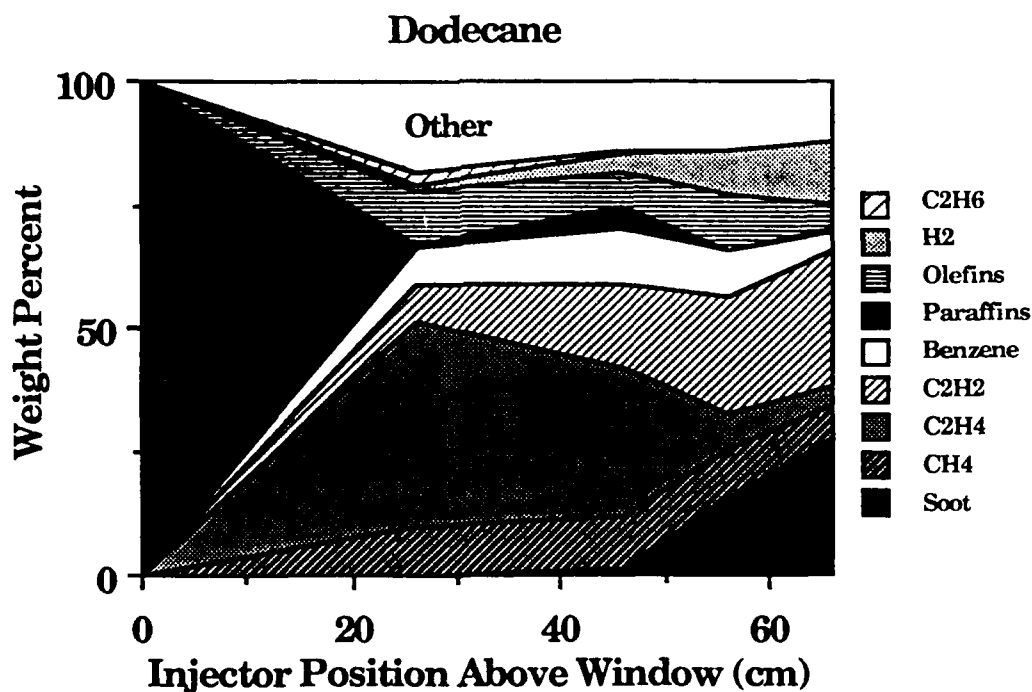
Dodecane

Figure 26. Pyrolysis Data for Dodecane as a Function of Injector Position at 1300°C. The Residence Time is Approximately 10 ms per cm.
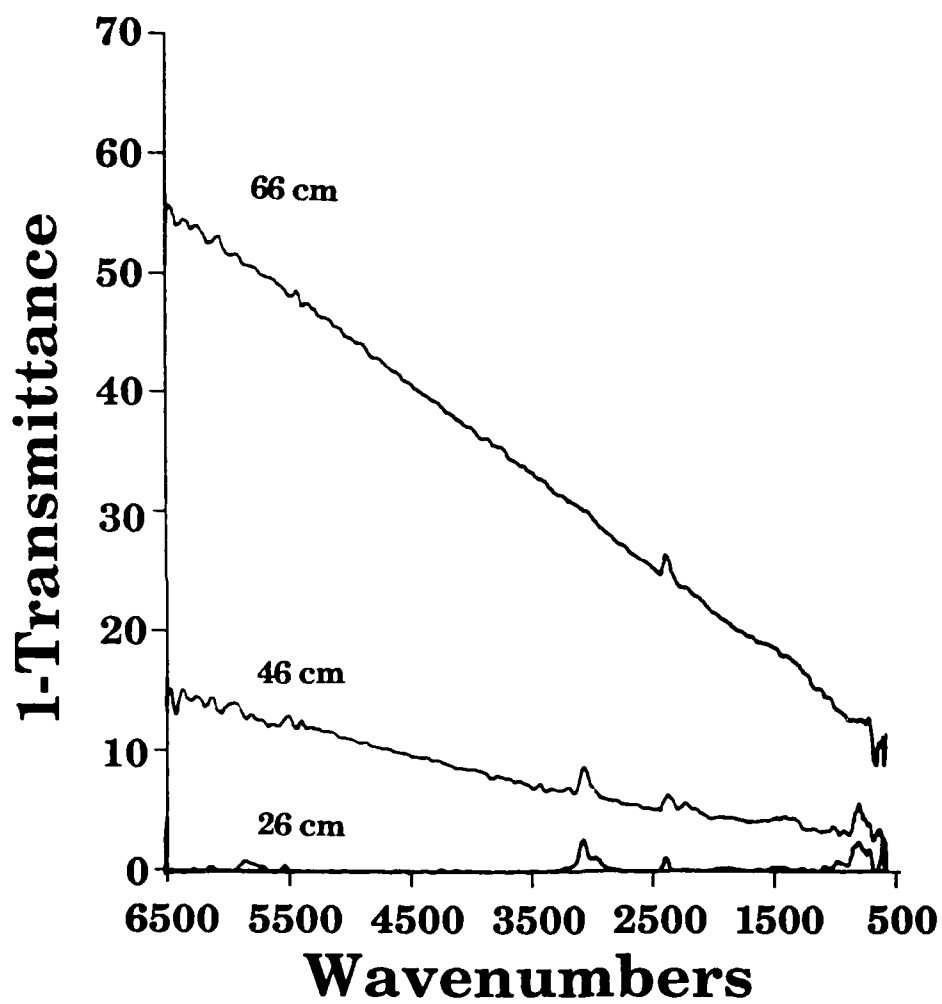
Figure 27. In-Situ 1-Transmission Experimental Data for Tetralin Taken During Mass Experiments of Fig. 11.
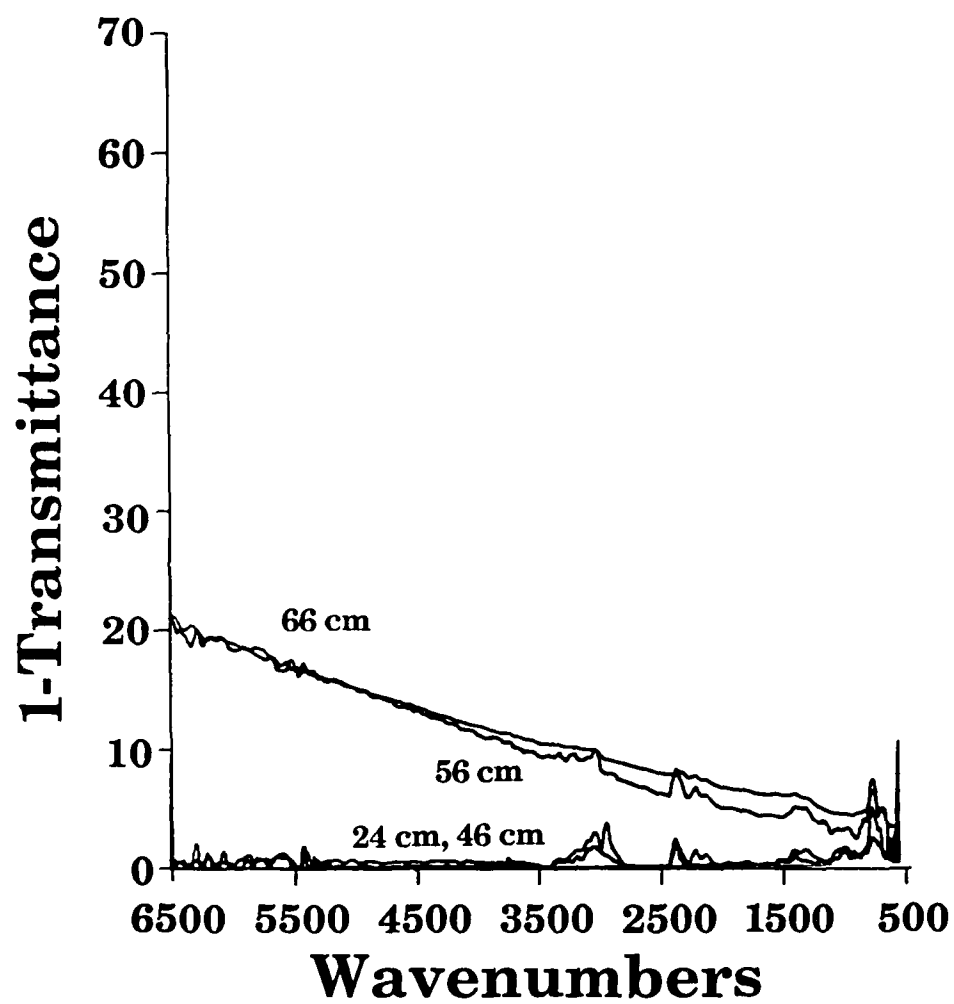
Figure 28. In-Situ 1-Transmission Experimental Data for Decalin Taken During Mass Experiments of Fig. 12.
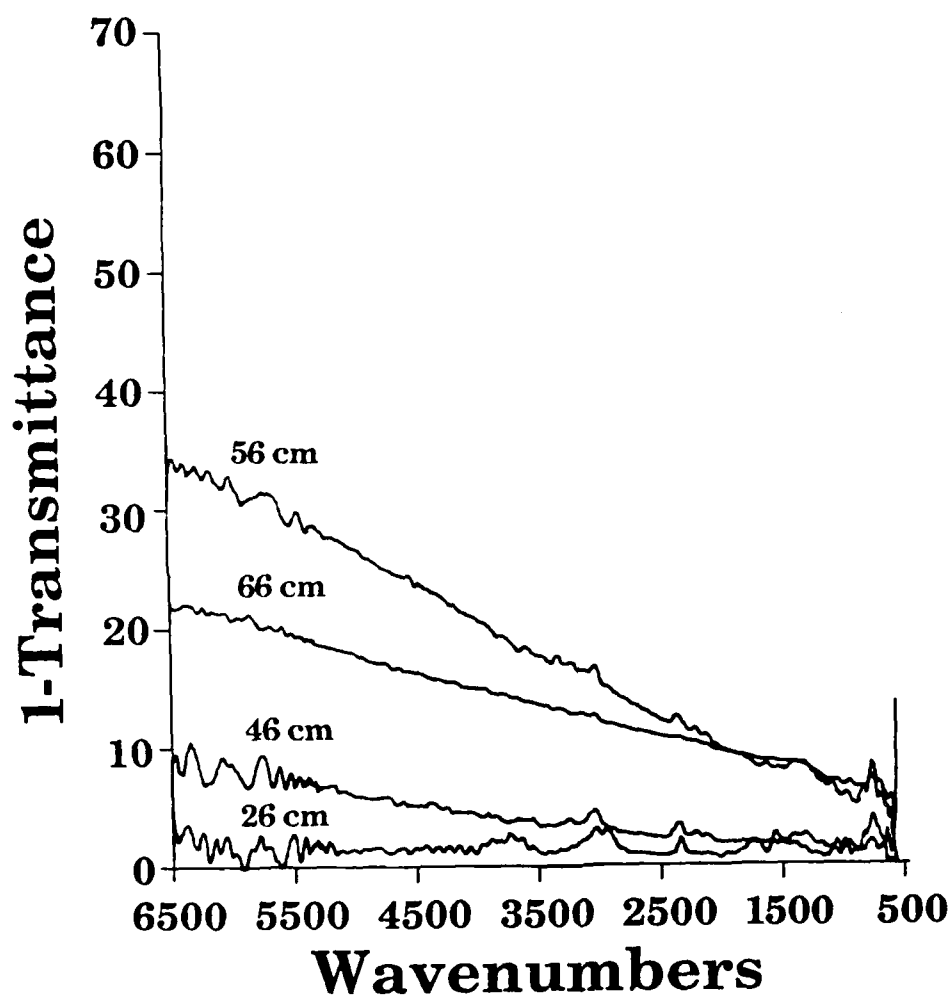
Figure 29. In-Situ 1-Transmission Experimental Data for JP8X-2414 Taken During Mass Experiments of Fig. 13.
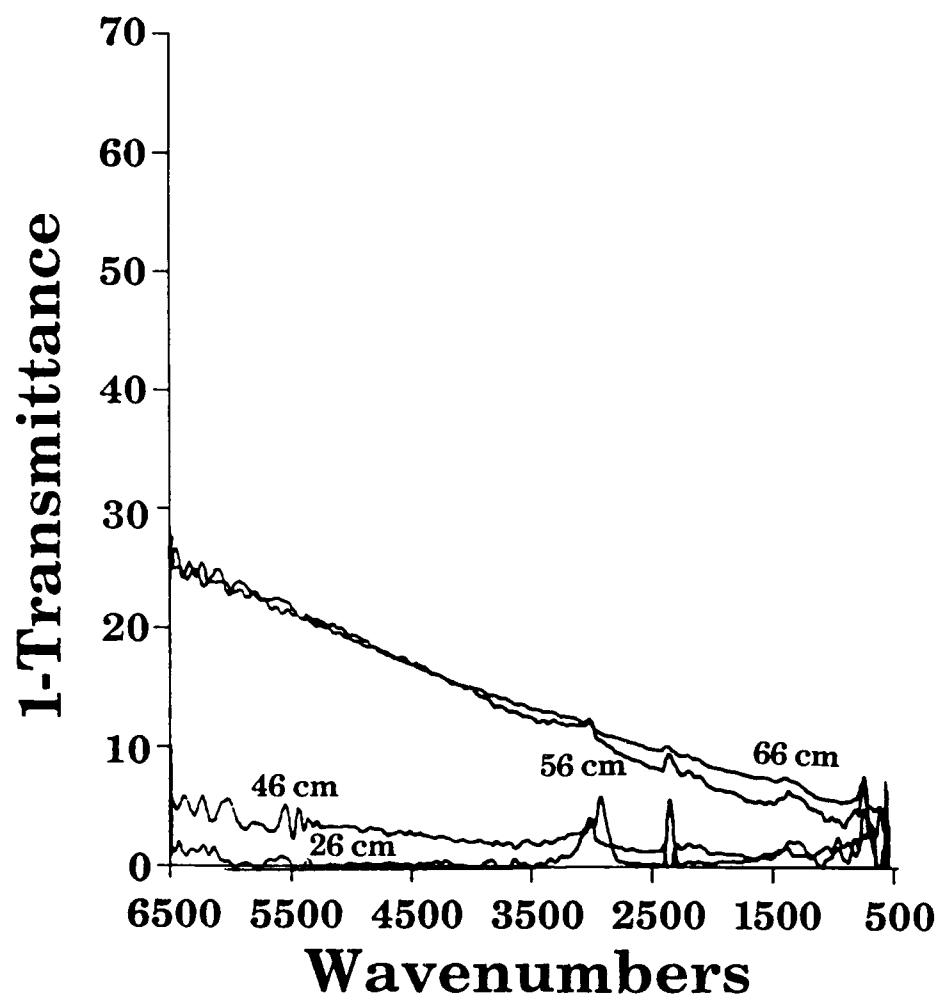
Figure 30. In-Situ 1-Transmission Experimental Data for JP8X-2383 Taken During Mass Experiments of Fig. 14.

The initial experiments with acetylene were contaminated with oxygen, which was traced to the solvent used to dissolve the acetylene in the tanks. This is true even for chromatography grade C_2H_2. The proprietary solvent used is apparently similar to acetone, or at least decomposes to acetone and was the source of the oxygen. The 1100 and 1500°C acetylene experiments were contaminated, but are included in the report for completeness.

In the course of tracing this contamination, we found that most of it could be removed using the appropriate traps (21,22). The 1300°C C_2H_2 experiments were made using the filtered acetylene.

There are several features common to all these data: The initial fuel cracks to form acetylene, hydrogen and ethylene. These species then recombine to form benzene, PAH's and soot. Pure benzene and acetylene are the major exception to this rule, and even in this case these light aliphatics appear with the soot. This observation led us to use a free radical soot chemistry model (23-25) as the basis of our modelling work in Task IV.

Emission/Transmission Experiments

The experimental results of the emission/transmission experiments are shown in Figs. 27 through 48. These are in the same order as listed in Table 2. For 13 of the mass balance experiments, in-situ transmission scans were taken during the pyrolyses as indicated in the 3rd column of the table. These are shown in Figs. 27 through 36. These figures all show the same trends: an increasing sloping baseline with increasing soot formation with a simultaneous disappearance of the identifiable gas bonds. Interestingly, several of the fuels (tetralin, Fig. 27 and JP8X, Fig. 29, for example) show a clearly increasing amount of soot absorption with increasing pyrolysis time, while others (decalin, Fig. 28, or JP8X-2398, Fig. 31) do not. Some of this may be due to spectrometer alignment, but the reproducibility indicates otherwise.

These spectra, where the 66 cm absorption is less than that for the 56 cm case may indicate agglomeration of the soot into the size range > 0.3 μm. Even if the soot is a fluffy chain of aromatics, the relevant size is the overall size of the cluster, although its optical density may be reduced by being some combination of N_2 gas and PAH rather than being all hydrocarbon. This could have the results of reducing the 1-τ_ν (due to leaving the Rayleigh regime where the absorption goes
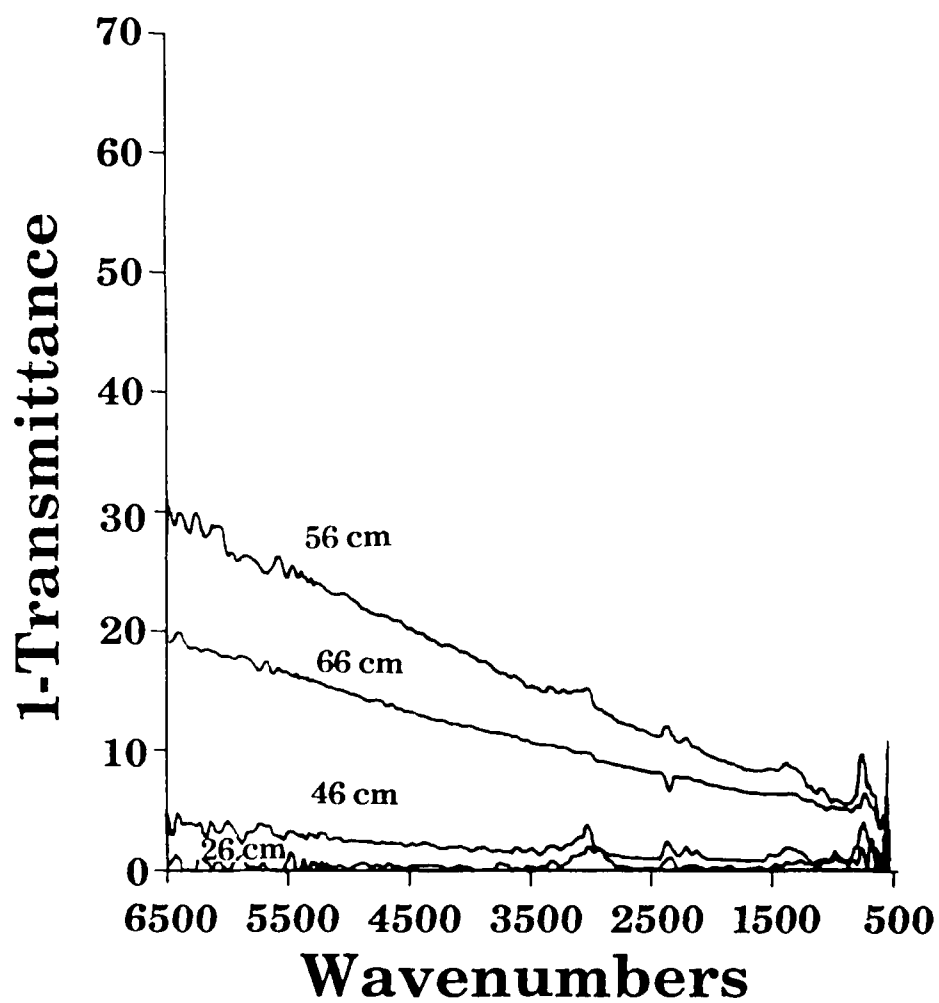
Figure 31. In-Situ 1-Transmission Experimental Data for JP8X-2398 Taken During Mass Experiments of Fig. 15.
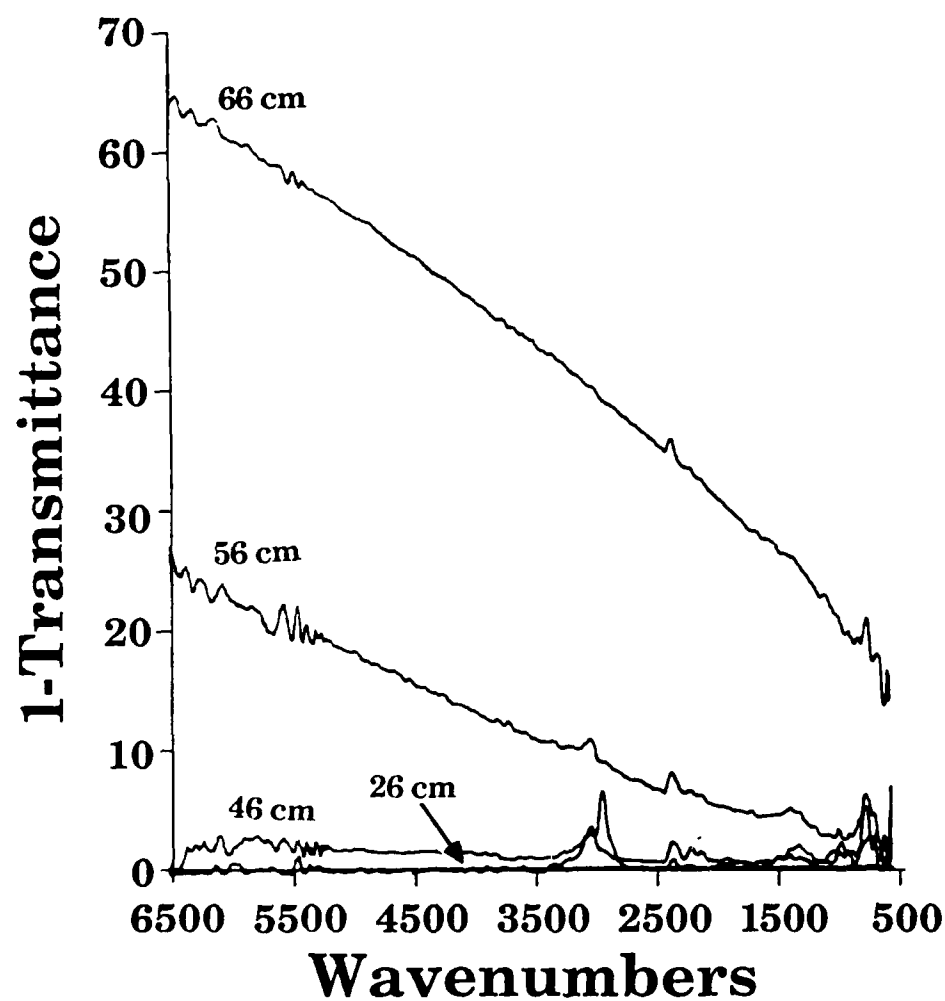
Figure 32. In-Situ 1-Transmission Experimental Data for JP8X-2429 Taken During Mass Experiments of Fig. 16.

from a volume effect to a surface area effect). This is discussed further below in conjunction with the in-situ E/T scans.

In-situ FT-IR 1-T scan for butane pyrolysis at 1100°C are shown in Fig. 33. Of interest are the peaks at 2000-1700 cm^{-1} and below 1000 cm^{-1} which can be assigned to aromatic and substituted aromatic species. These are clearly present by 26 cm. **The presence of these species at a reaction point where acetylene is at very low concentration may indicate that PAH precursors are also being generated by a reaction pathway that does not involve acetylene as a basic building block in ring formation.** However, the modeling work in Task VI indicates that this is probably not a dominant effect for the low density experiments. At high pressures, where the molecular fragments are larger, it may be important. This possibility is discussed further in Section V.

In-situ FT-IR data for butane confirms the differences in soot content as established by mass balance. Figure 34 compares transmission measurements for each experiments of Figs. 18, 20 and 21. The sloping baseline indicative of small particle light extinction is clearly seen to change relative to injector distance, and also relative to H$_2$ or O$_2$ addition. At a reactor temperature of 1100°C, a sloping baseline shift was not observed since these experiments did not produce soot.

Figure 35 shows a series of FT-IR spectra for (1-transmission) and emission for pyrolysis of acetylene in the reactor at 1300°C. The spectra were accumulated over a series of reaction distances from 6 to 66 cm. The gas velocity is 1 meter/sec giving a maximum residence time of 660 msec. At short reaction distances, the transmission spectra show the acetylene bands alone. The amplitude of the absorbance for this series was shown to be proportional to the amount of soot collected. The spectra illustrate the ability to obtain soot and gas concentrations in the same measurement.

Figure 35b presents the emission spectra for the same series. The spectra show the features corresponding to those in the transmission spectra but are lower in noise. At short reaction distances, the emission spectra show the acetylene bands. The spectra increase in amplitude as the acetylene heats. At about 26 cm a small bump is observed at (3100 wavenumbers) on the side of the acetylene emission. This is in the aromatic C-H stretch, from PAH precursors. The aromatic C-H stretch grows with increasing distances. At about 30 cm, a broad emission is observed due
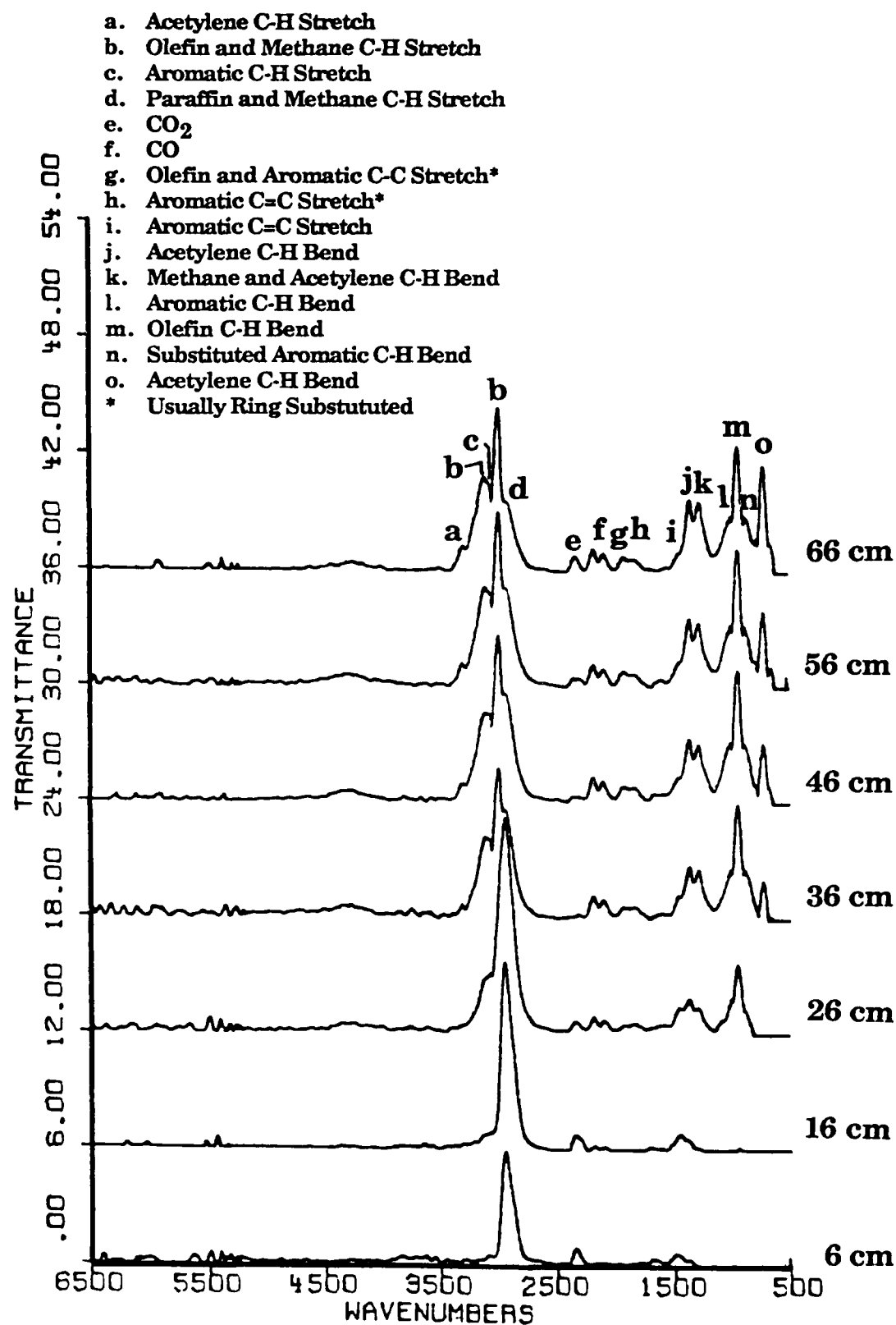
Figure 33. 1-Transmission Spectra for Butane Pyrolysis (1100°C) at Variable Reaction Distances. Spectra are Offset for Display Purposes. This Data was Taken During Experiments of Fig. 17.
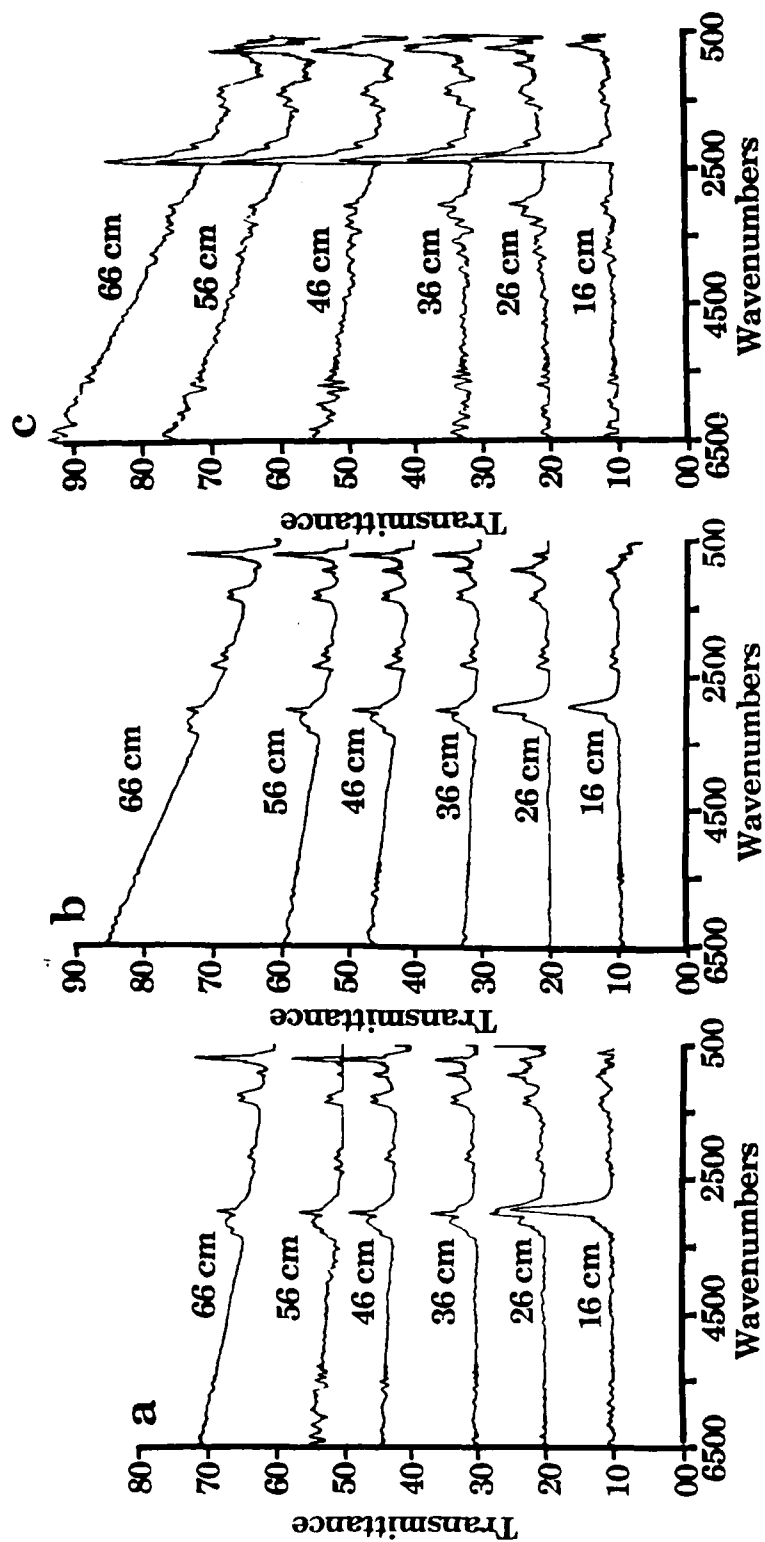
Figure 34. 1-Transmission Spectra for Butane Pyrolysis (1300°C) at Variable Reaction Distances. Spectra are Offset for Display Purposes. a) Butane+H$_2$ Addition, b) Butane and c) Butane+O$_2$ Addition. These are the Same Experimental Runs as Shown in Figs. 20, 18, and 21, Respectively.
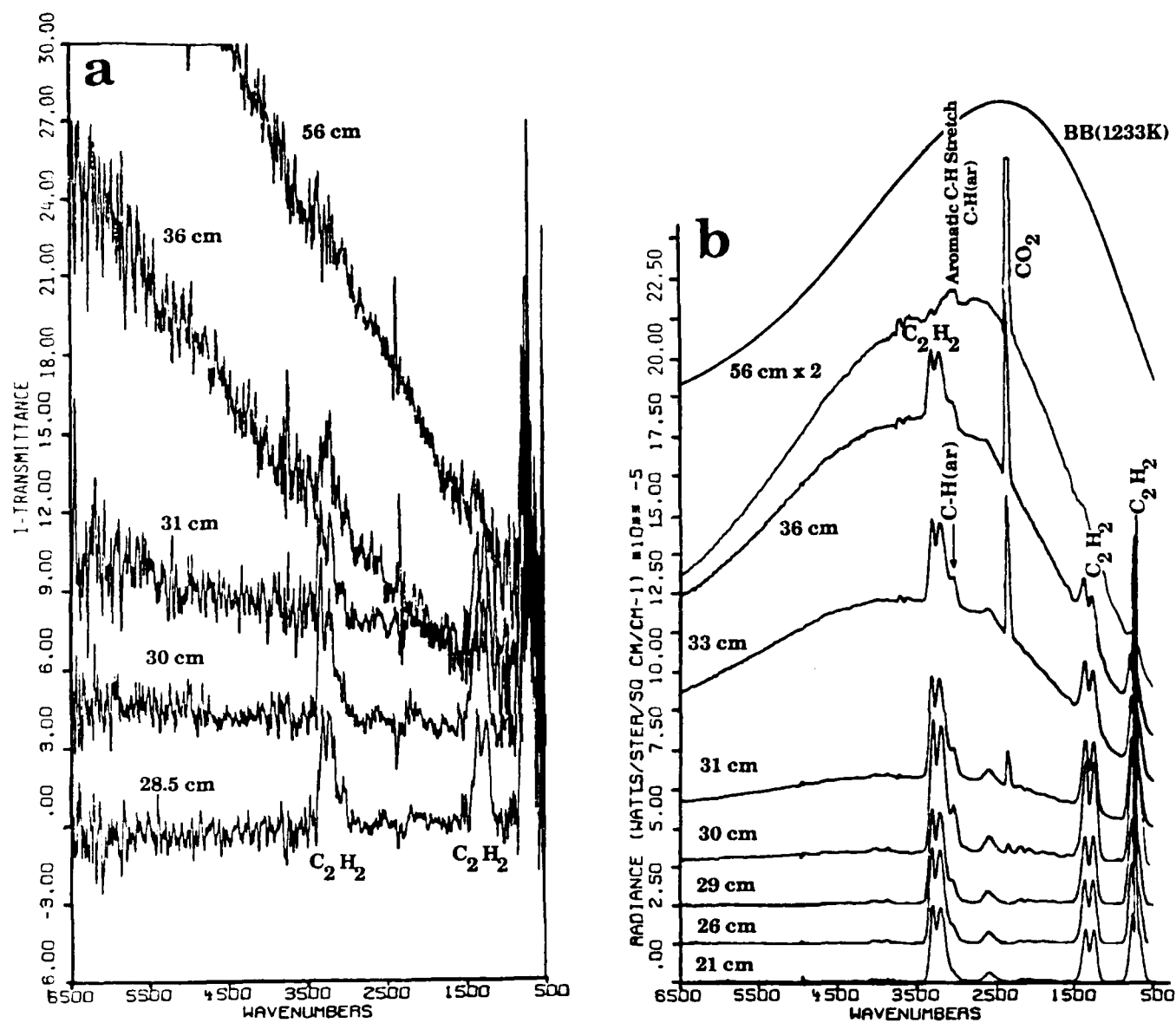
Figure 35. In-Situ Experimental Data for Acetylene as a Function of Injector Position. This is for the "contaminated" Experiments (see text). a) 1-Transmission and b) Emission.
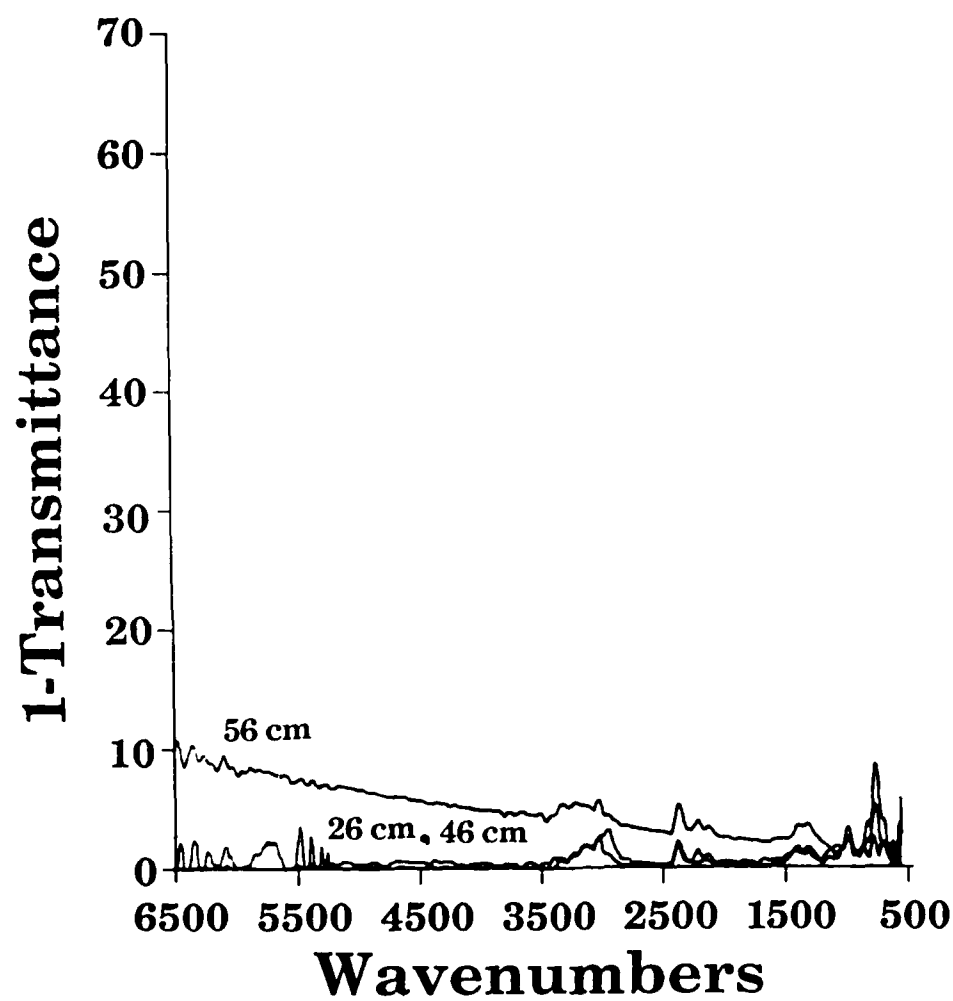
Figure 36. In-Situ 1-Transmission Experimental Data for Tetralin Taken During Mass Experiments of Fig. 26.

to soot. This broad peak grows while the acetylene emission decreases as the acetylene is consumed. The aromatic C-H stretch peak remains, even for the longest reaction distance.

In addition to the in-situ transmission scans during mass balance experiments, 19 of the fuels were pyrolyzed at 66 cm (maximum residence time), at various temperatures, and with added H_2 or O_2, as indicated in the last column of Table 2. During these pyrolyses, the emission and transmission were measured as discussed in Section II. The full mass balances were not measured during these experiments.

For each fuel in these E/T experiments, Figs. 37 through 54 show a) the measured 1-Transmission, b) the radiance R_ν(Eq. (4)) and c) the normalized radiance (Eq. (7)). Since the emission or radiance measurement was taken after the transmission measurement, the normalized radiance computation helps to provide a consistency check on the two measurements; since if the experimental conditions change, the normalized radiance will no longer be a black-body curve.

In the cases where more than one experimental condition was measured, all the results for one fuel are plotted on the same figure to emphasize the changes. Of interest is the variation with H_2 or O_2 addition: the addition of 7.2 vol% H_2 always reduces the emission, (and increases the transmission) indicating a reduction of soot. Conversely, the addition of O_2 increases the soot. We attribute this to the capping of radical soot precursors by the presence of hydrogen, or the consumption of hydrogen by the oxygen.

In an effort to correlate the quantity of soot implied by the emission, with that measured in separate mass balance experiments, we plot in Fig. 55a, the measured soot vs $1-\tau_\nu$ at 6500 cm^{-1}. As can be seen, the correlation is poor. This can be caused by several factors. One possible factor is that since the actual soot quantities, and the in-situ radiance were measured in different runs on different days, there could be day-to-day variations in experimental conditions which caused variations in the amounts of soot generated. Repeat experiments on several of the runs, however, showed good reproducibility in both the mass balance and the E/T data, indicating that this is not a major factor.

A second source of error in Fig. 55 could be in the emissivity of the soot, assumed to be constant. If the emissivity differs among the soots produced from different fuels, or the soots have aged differently, the radiance or $1-\tau_\nu$ will not be a qualitative measure of the soot.
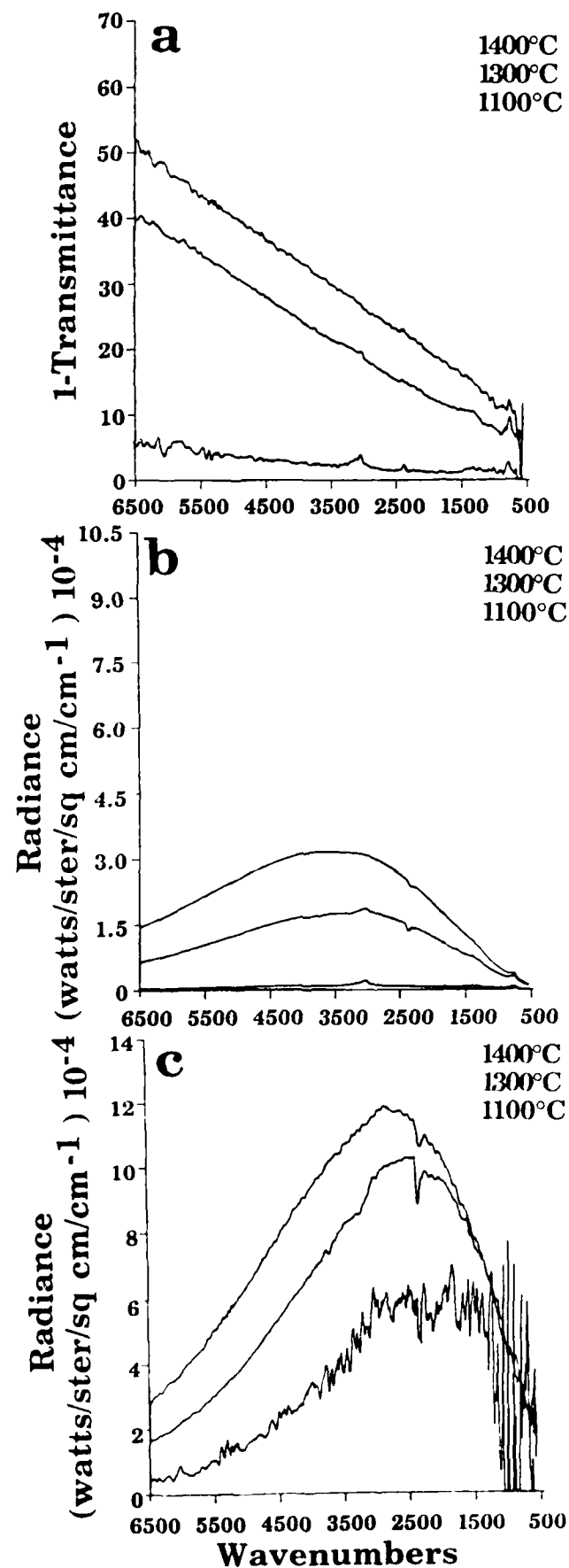
Figure 37. Fuel UTRC-2A Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.
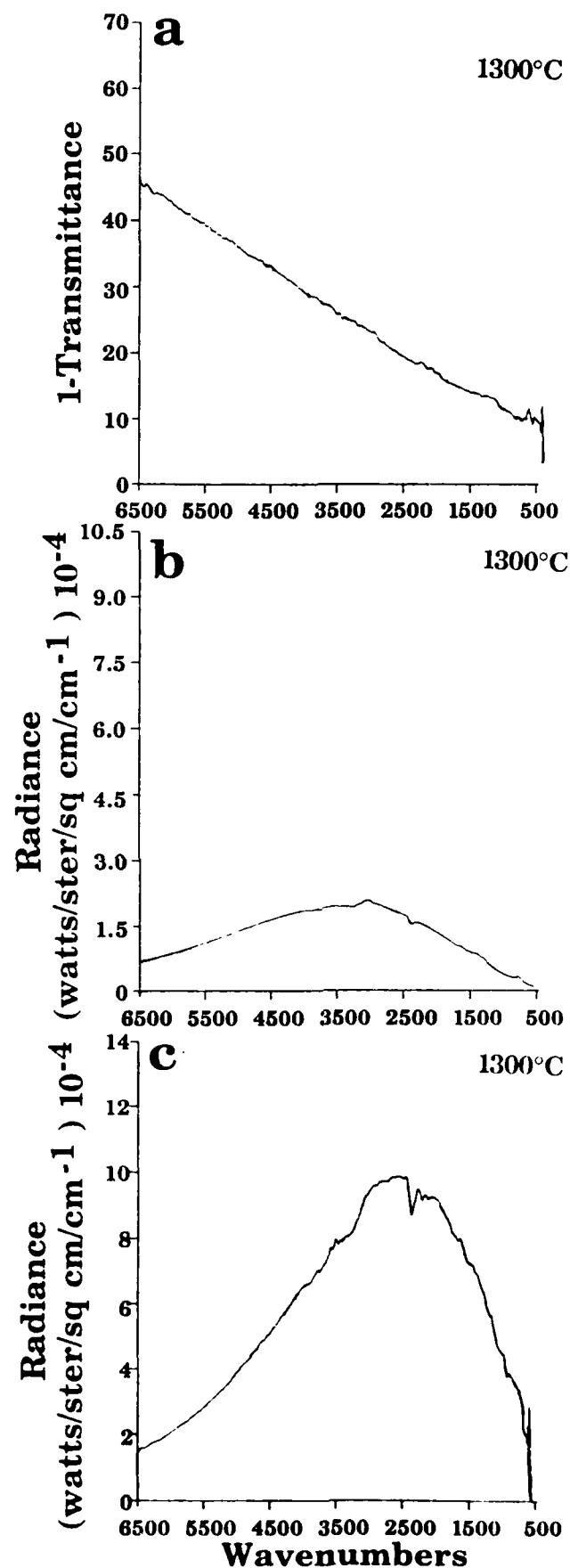
Figure 38. Fuel ERBLS-1 Pyrolyzed in the Entrained Flow Reactor
for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and
c) Normalized Radiance. The Legends are in Order of the Curves.
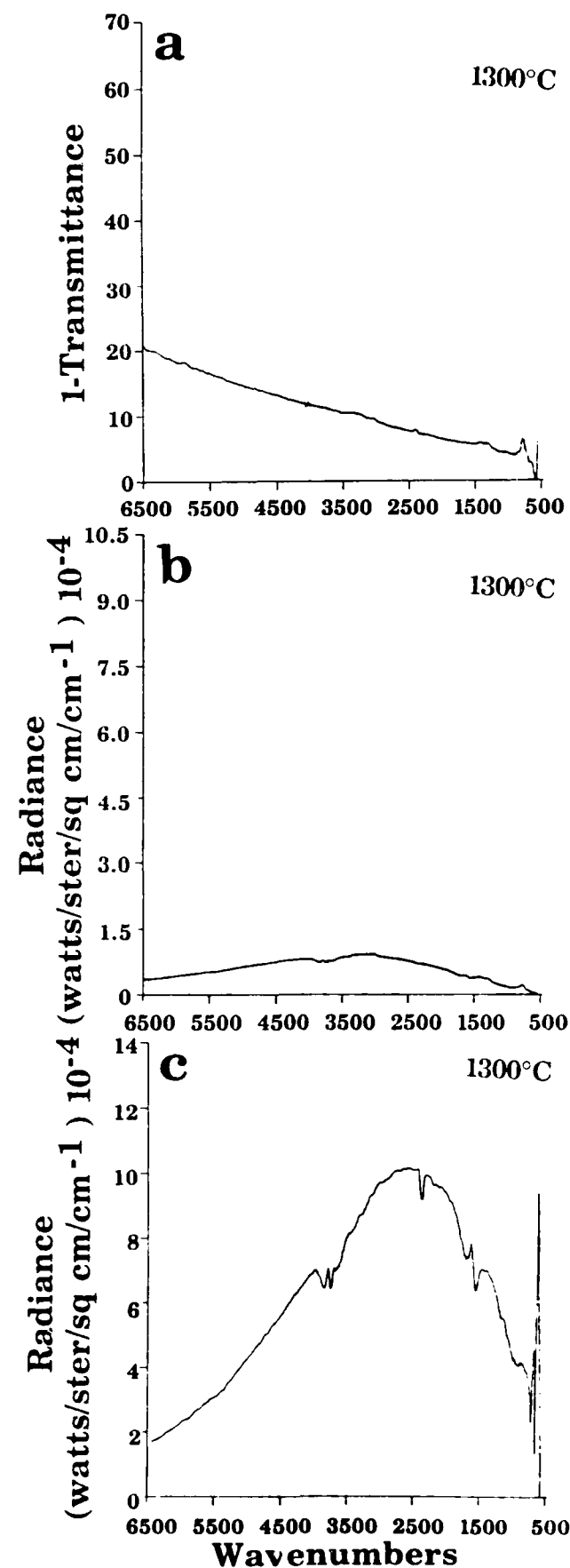
Figure 39. Fuel JP-7 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.

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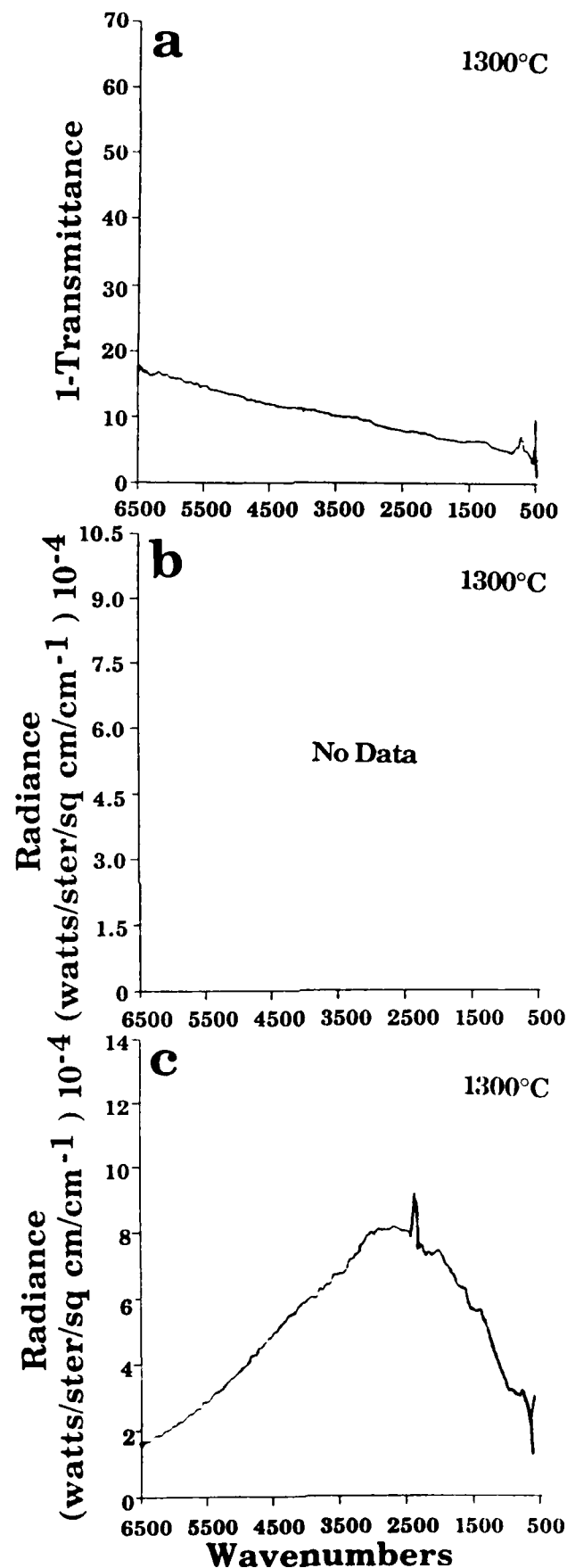
Figure 40. Fuel JP-4 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.
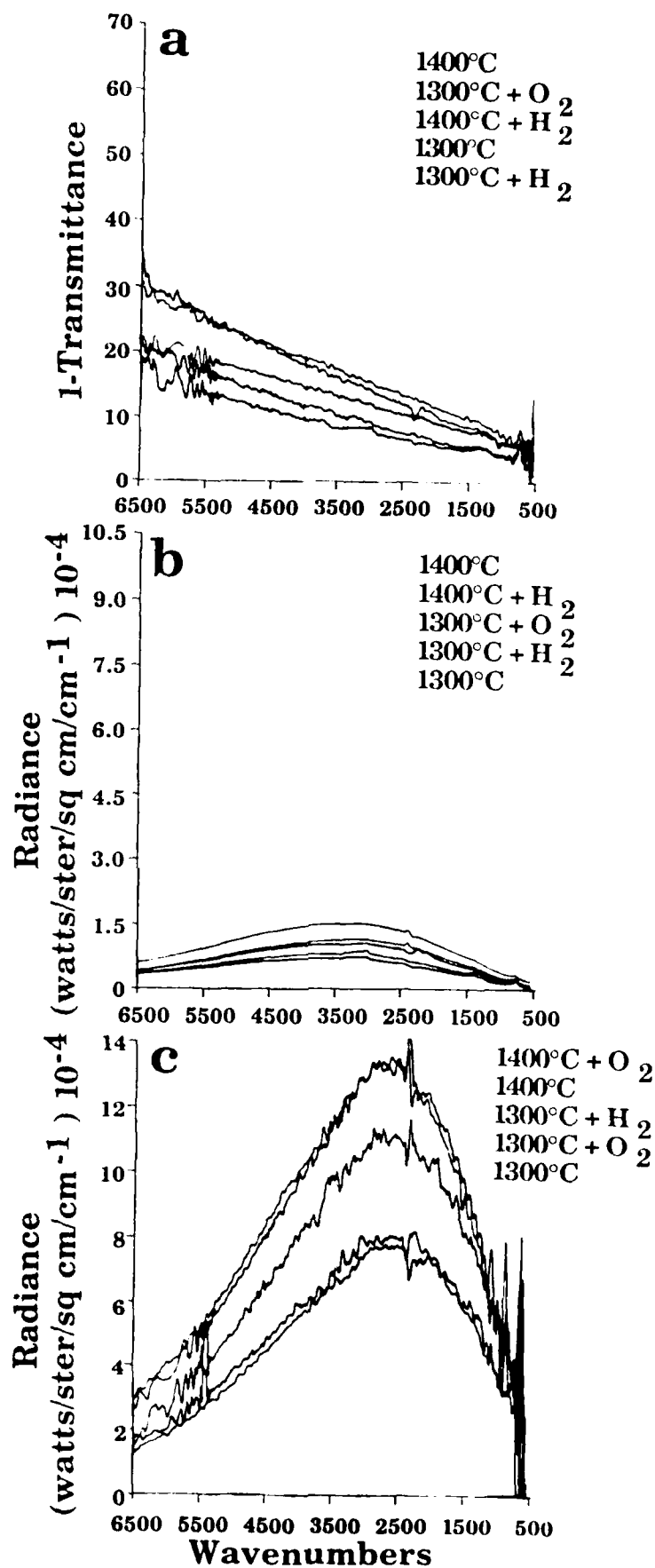
Figure 41. Fuel DF-2 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.
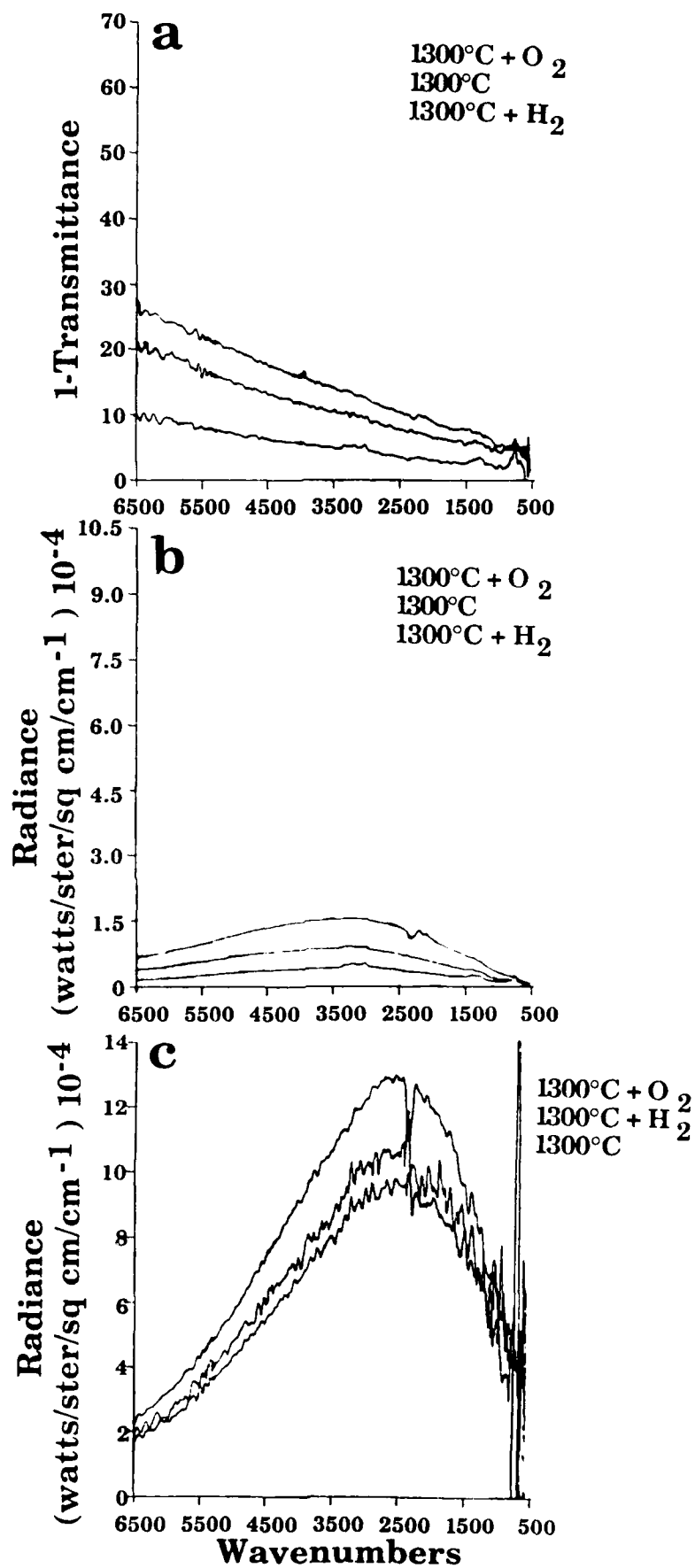
Figure 42. Fuel AFAPL-6 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.
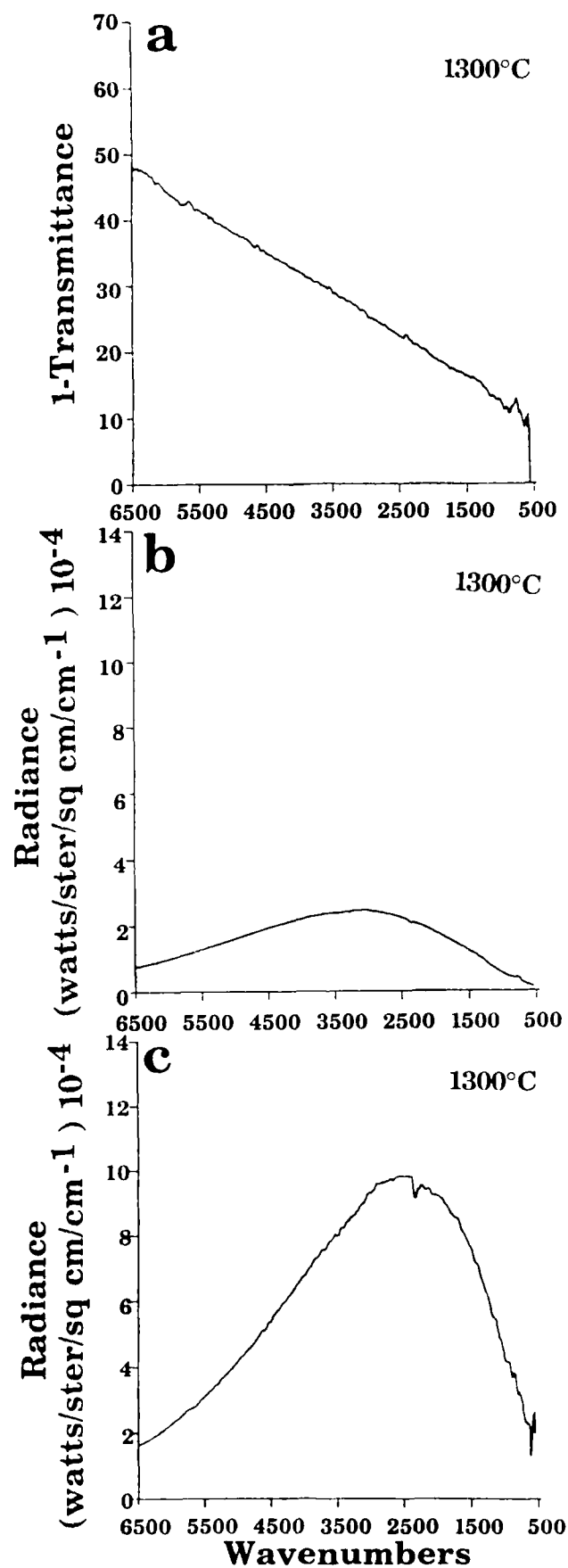
Figure 43. Fuel AFAPL-2 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.
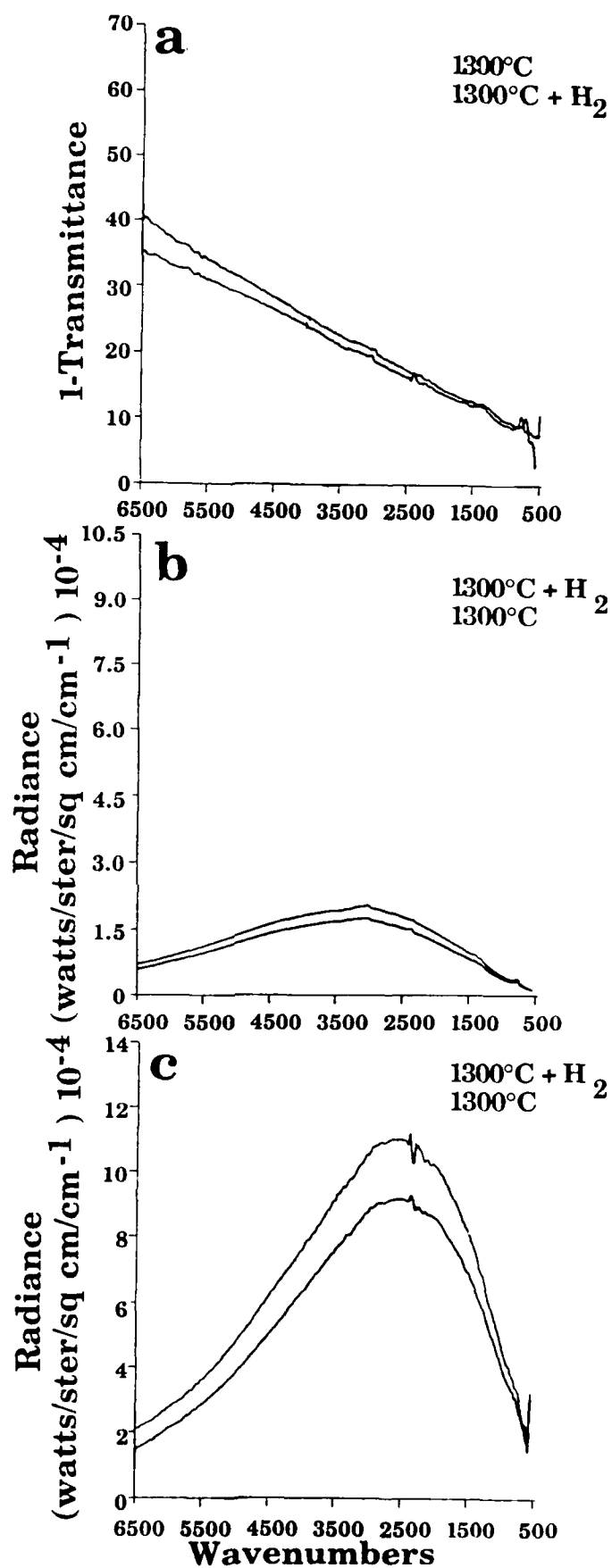
Figure 44. Fuel ERBLS-2 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.

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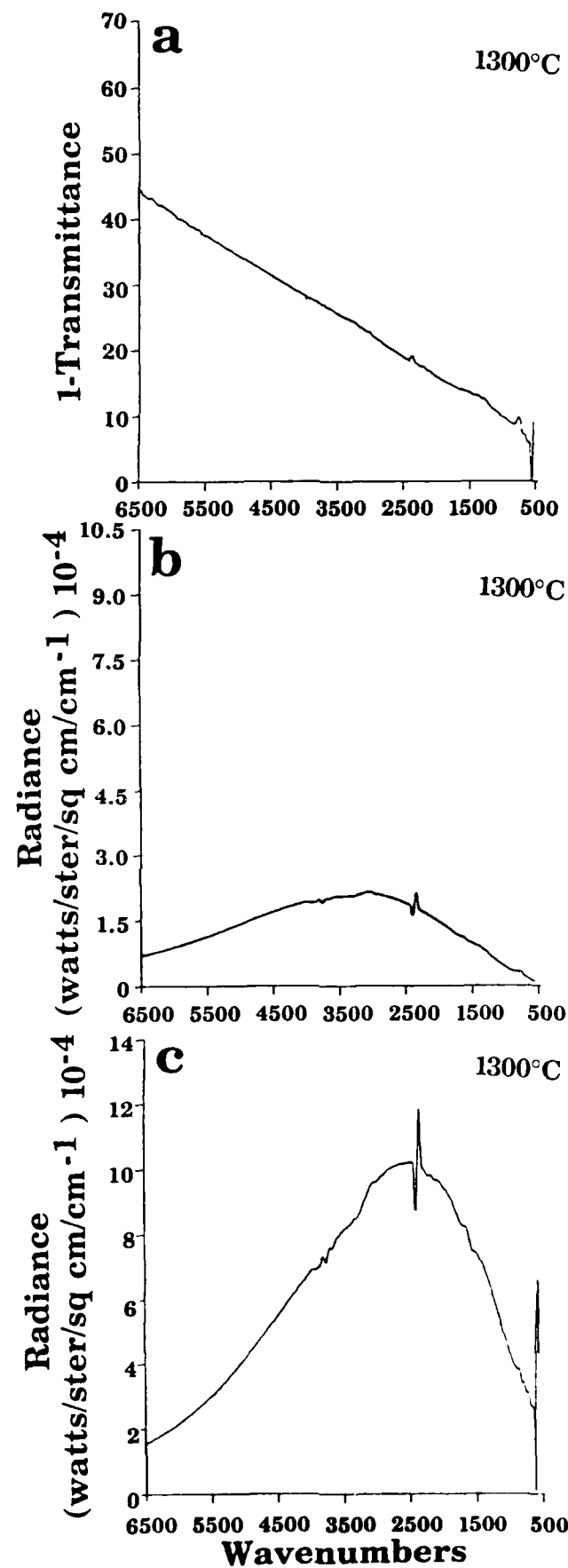
Figure 45. Fuel UTRC-9A Pyrolyzed in the Entrained Flow Reactor
for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and
c) Normalized Radiance. The Legends are in Order of the Curves.
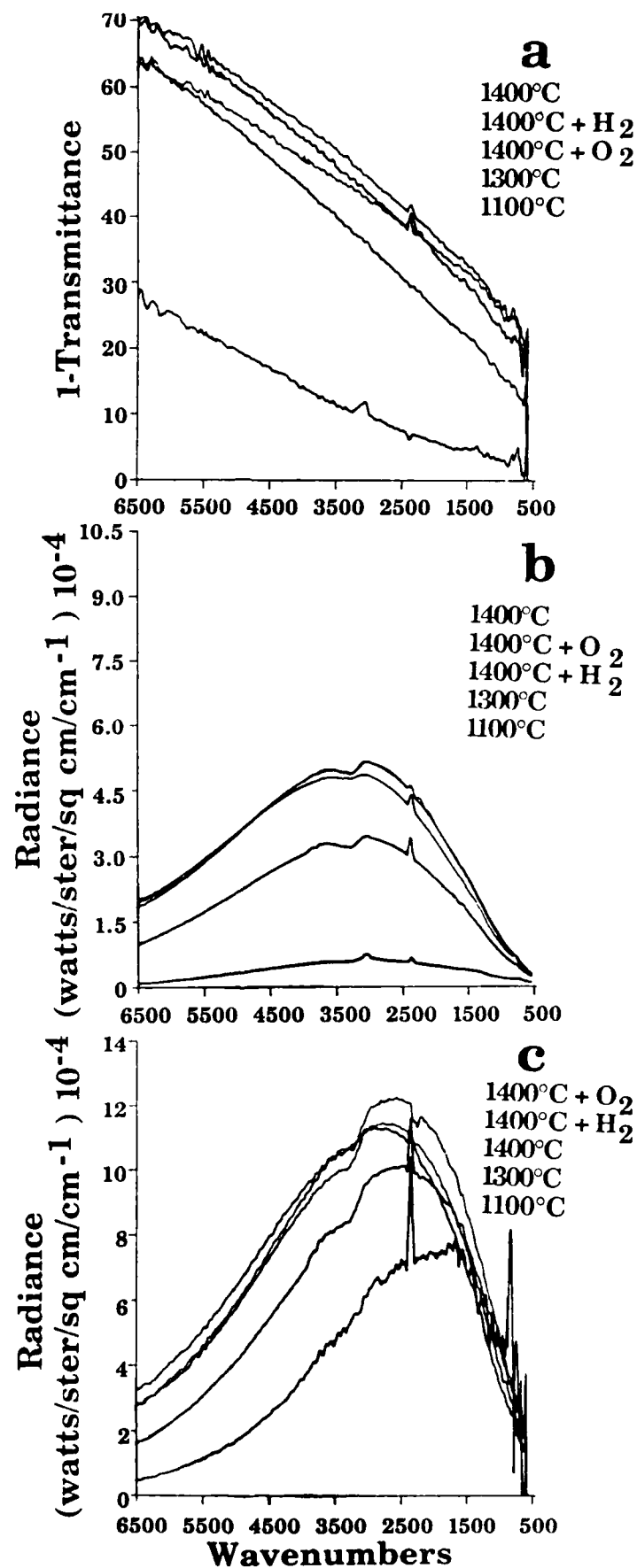
Figure 46. Fuel XTB Pyrolyzed in the Entrained Flow Reactor for a
Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and
c) Normalized Radiance. The Legends are in Order of the Curves.
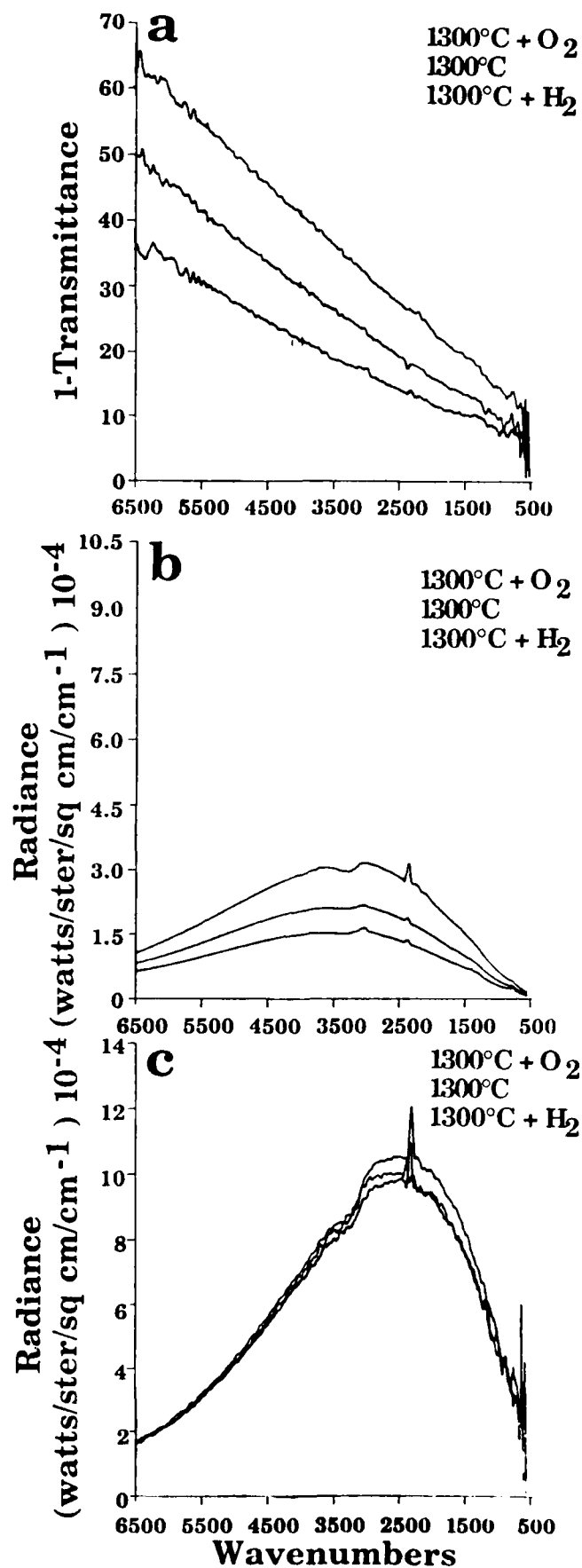
Figure 47. Fuel BLS Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.
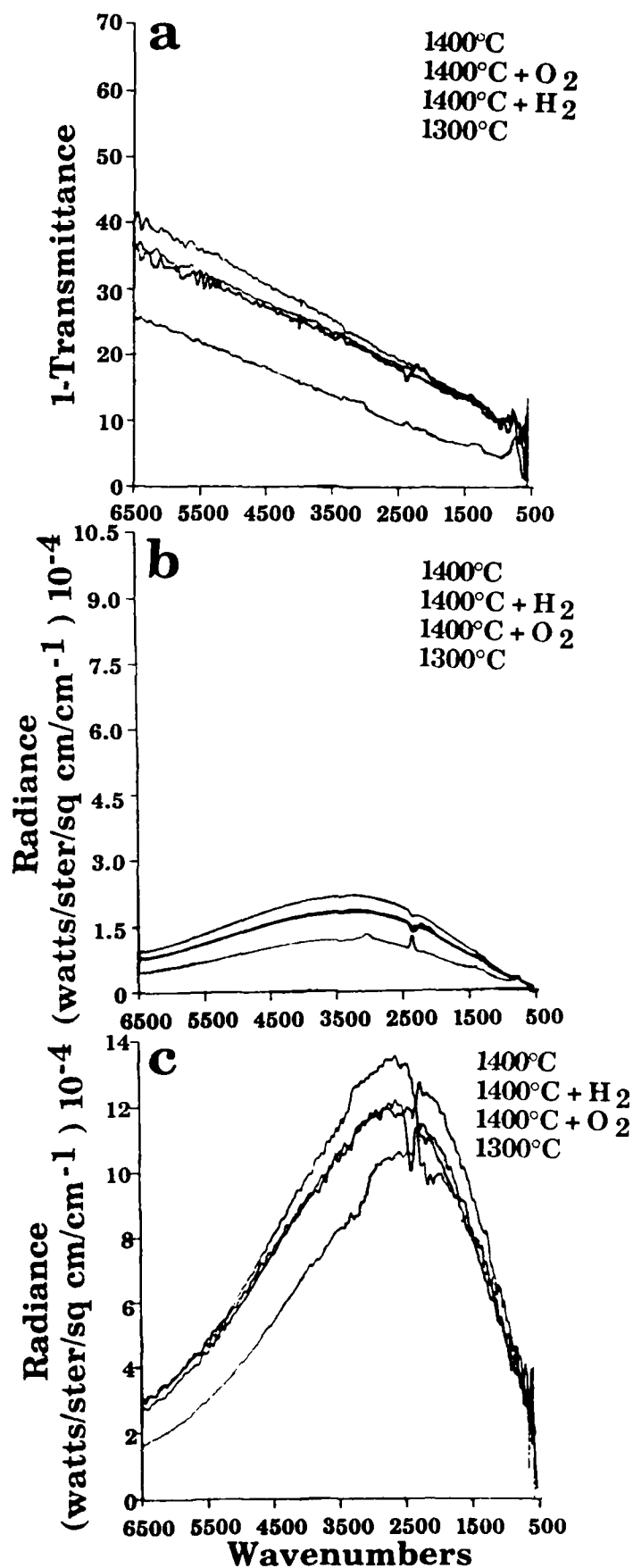
Figure 48. Fuel Decalin Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.

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a

1300°C + O$_2$
1300°C
1300°C + H$_2$

(y-axis: 1-Transmittance, 0–70; x-axis: 6500 5500 4500 3500 2500 1500 500)

b

1300°C + O$_2$
1300°C
1300°C + H$_2$

(y-axis: Radiance (watts/ster/sq cm/cm^{-1}) 10^{-4}, 0–10.5; x-axis: 6500 5500 4500 3500 2500 1500 500)

c

1300°C + H$_2$
1300°C
1300°C + O$_2$

(y-axis: Radiance (watts/ster/sq cm/cm^{-1}) 10^{-4}, 0–14; x-axis: 6500 5500 4500 3500 2500 1500 500)

Wavenumbers
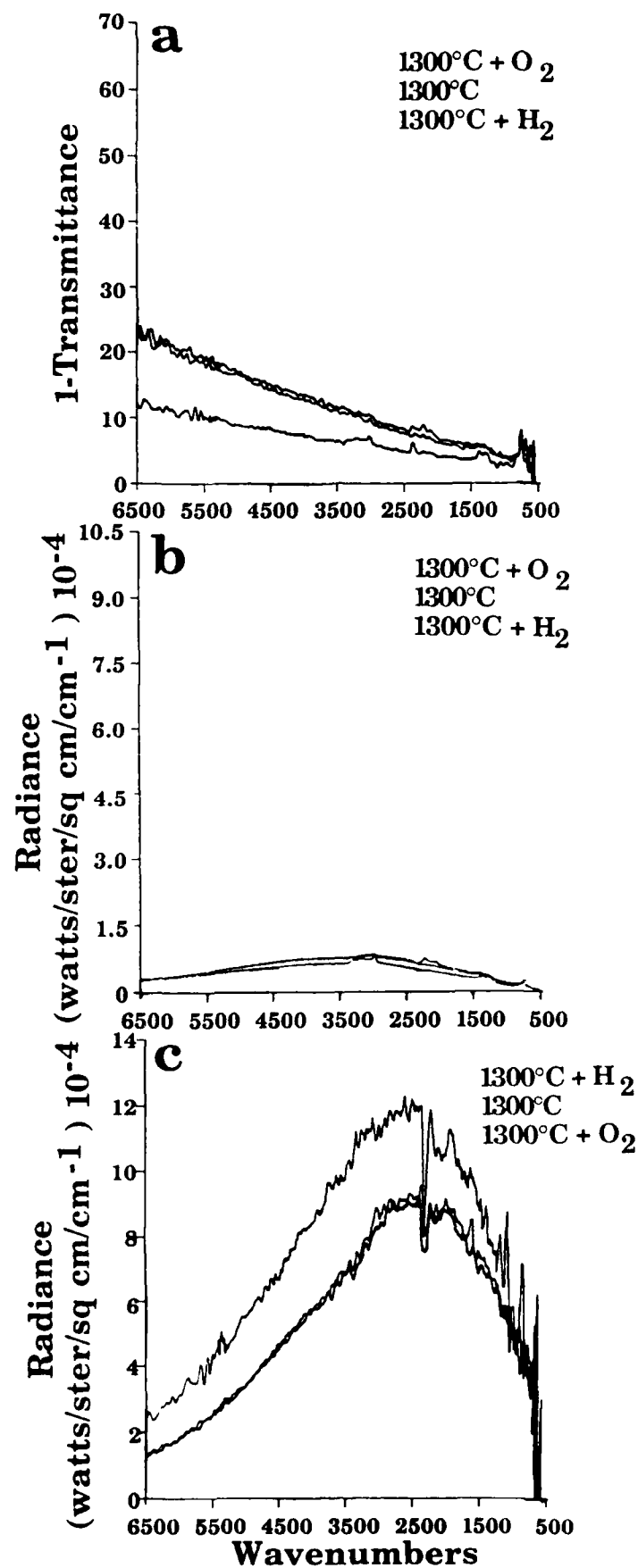
Figure 49. Fuel JET-A Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.

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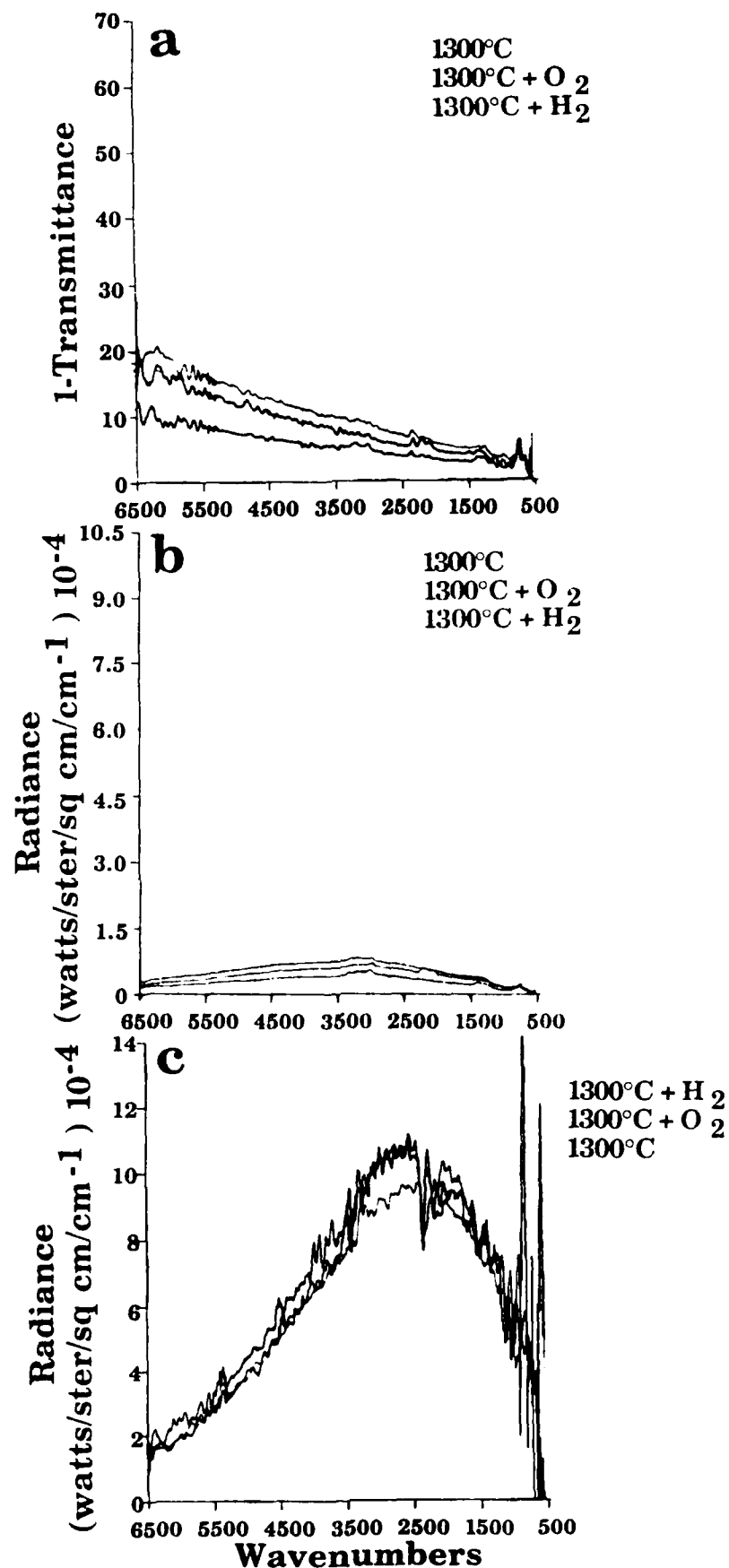
Figure 50. Fuel JP-5 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.
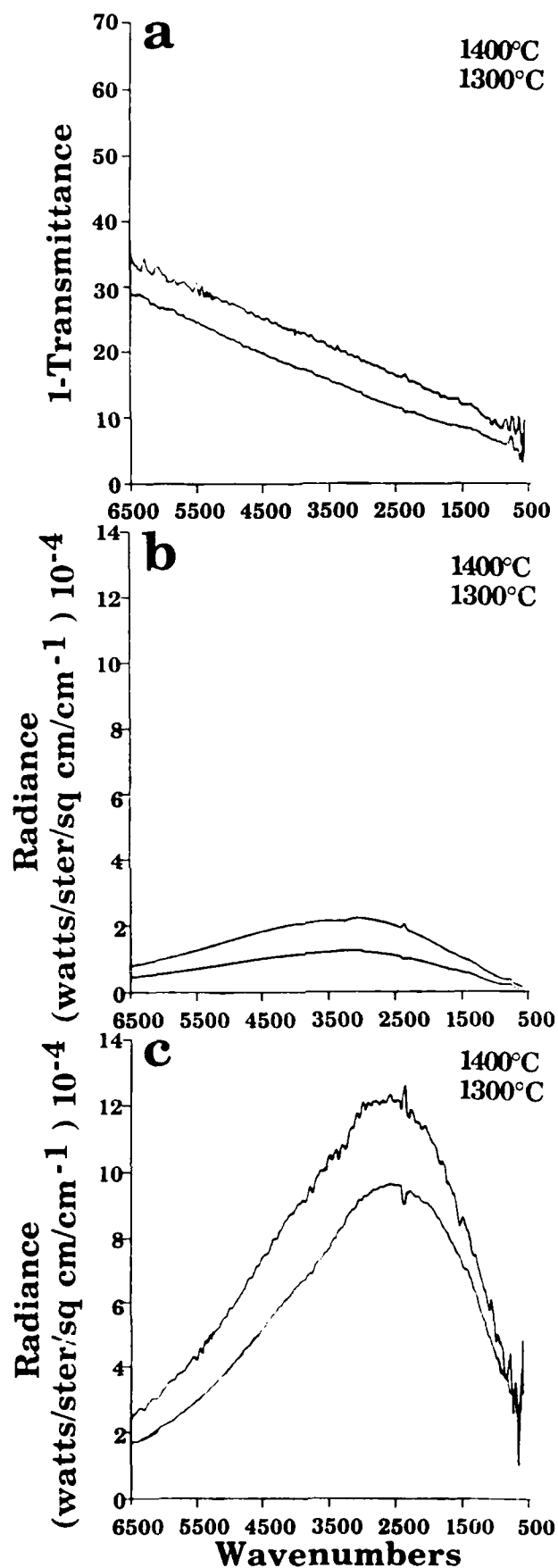
Figure 51. Fuel JP8X-2414 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.
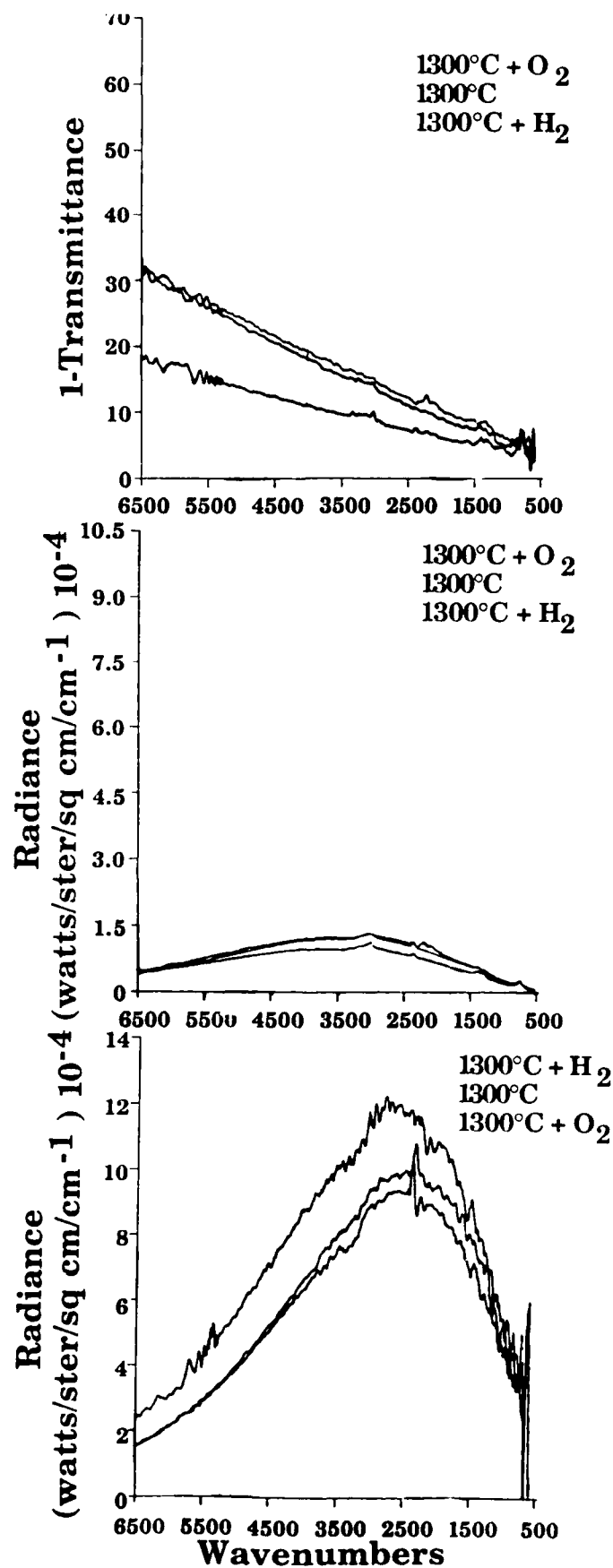
Figure 52. Fuel JP8X-2383 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.

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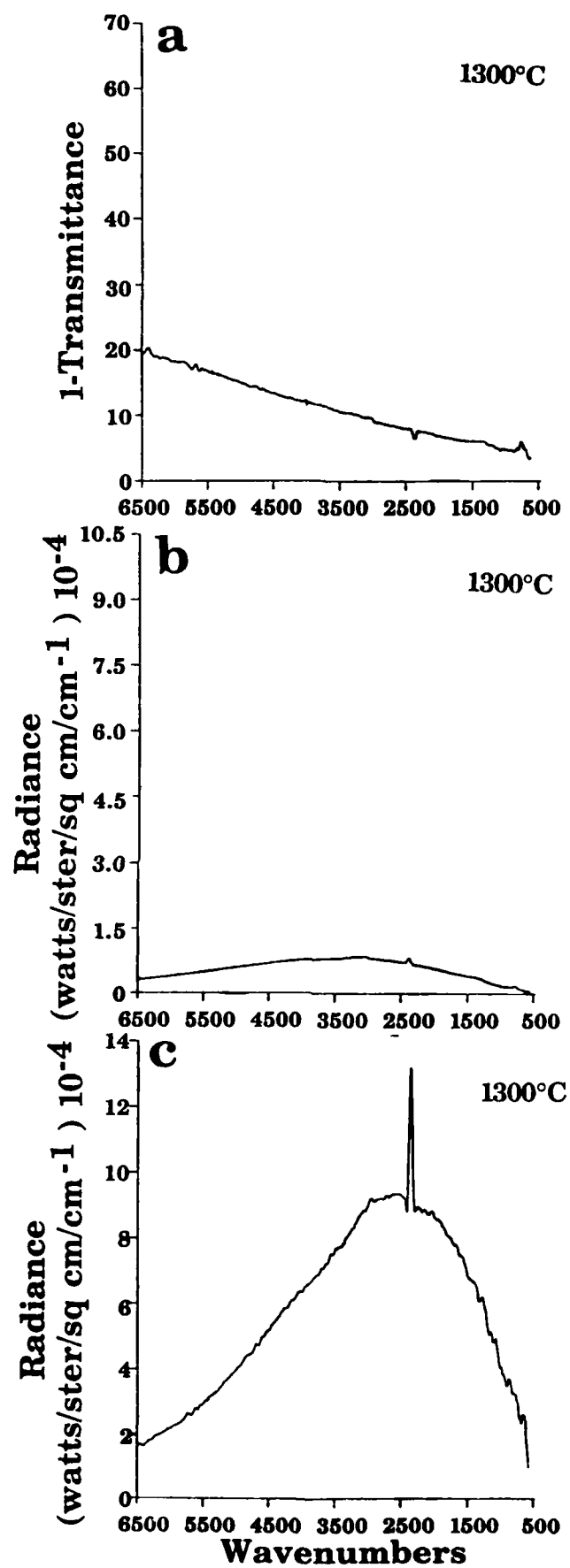
Figure 53. Fuel JP8X-2398 Pyrolyzed in the Entrained Flow Reactor
for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and
c) Normalized Radiance. The Legends are in Order of the Curves.
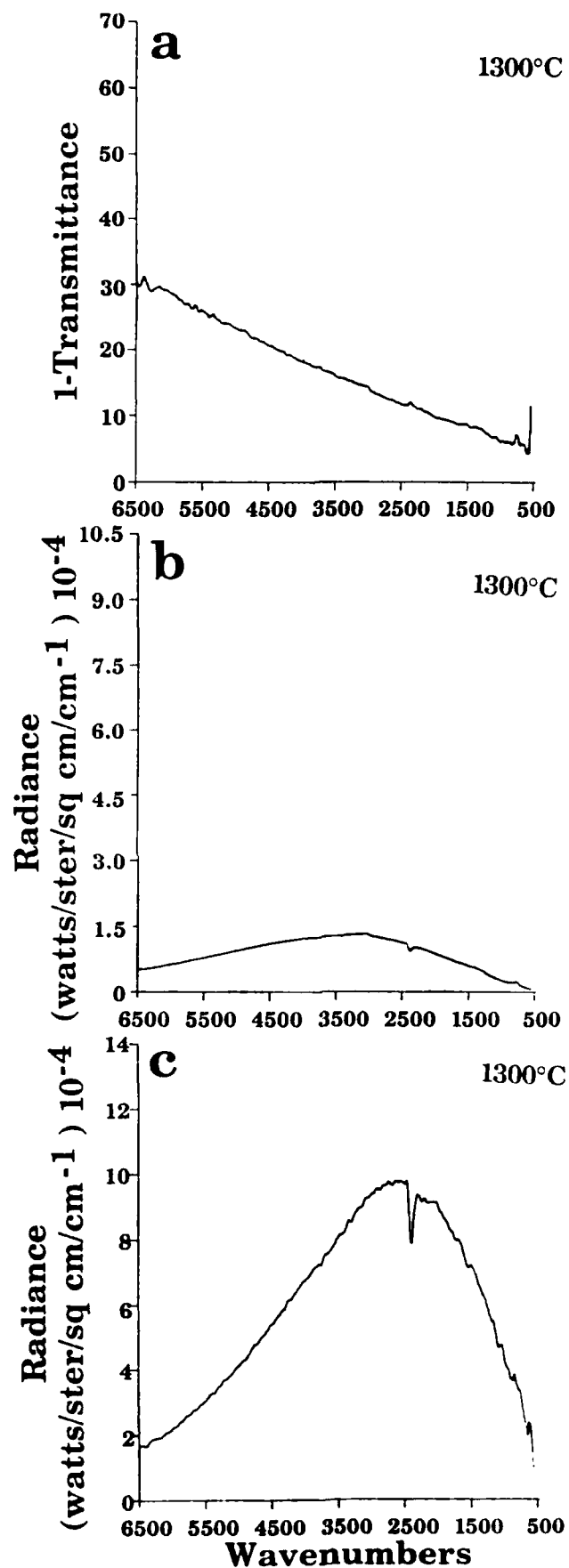
Figure 54. Fuel JP8X-2429 Pyrolyzed in the Entrained Flow Reactor for a Distance of 66 cm Reaction Distance a) 1-T, b) Radiance and c) Normalized Radiance. The Legends are in Order of the Curves.
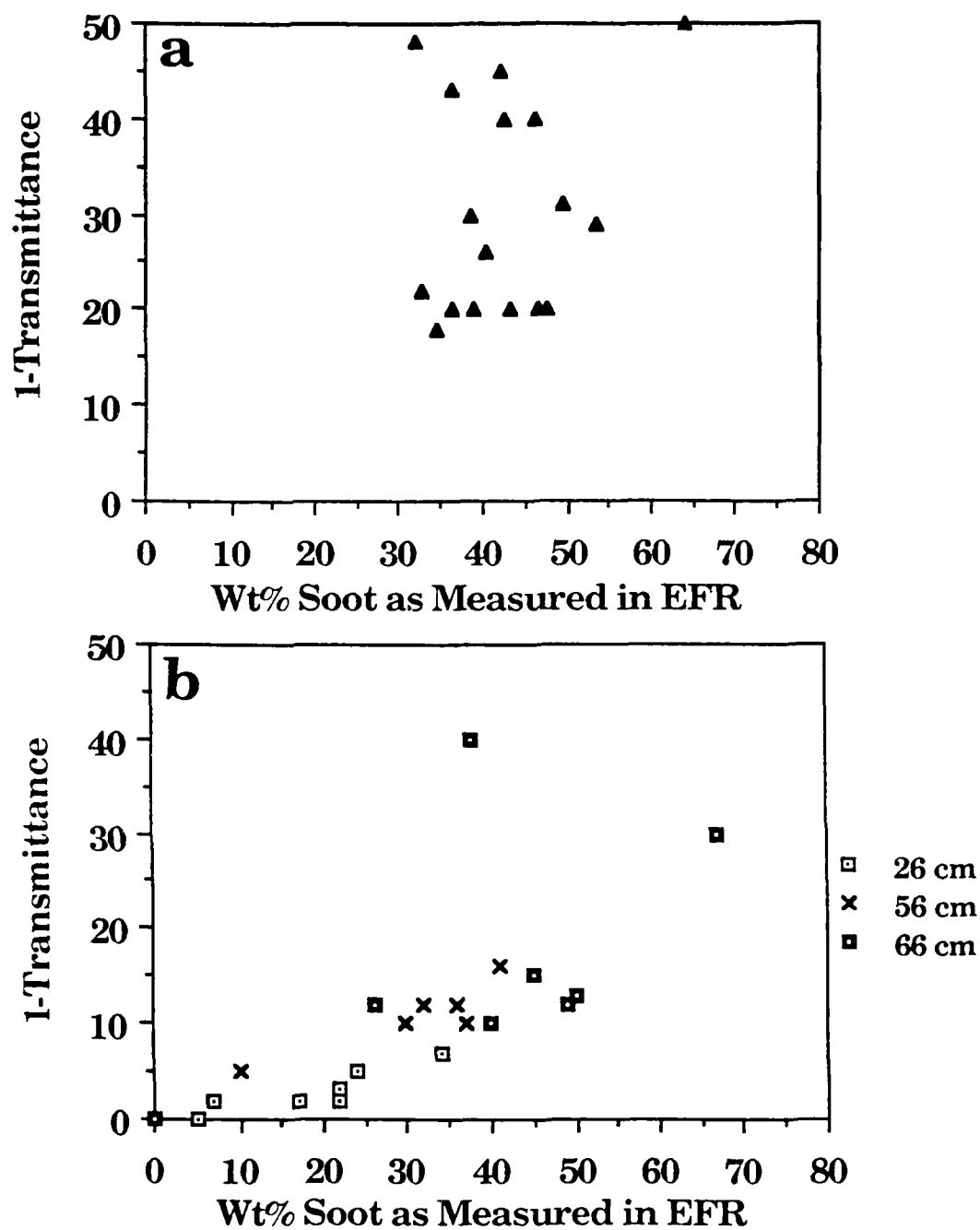
Figure 55. Correlation of 1-Transmission with Soot Measurements at 1300°C. a) 66 cm Data from Figs. 36 through 54 and b) Data for In-Situ Scans from Figs. 27 through 35.

As discussed in Section II, the $1-\mathcal{T}_\nu$ or the radiance for these young soots should be in the Rayleigh regime where the absorption is proportional to the volume fraction of soot and to a "constant" function of the optical constants. For very young soots, the optical properties may not be well developed, which would cause the extinction coefficient or $1-\mathcal{T}_\nu$ to be reduced below that for a more well developed (aged) soot. To test this possibility, in Fig. 55b and 55c we have plotted the $1-\mathcal{T}_\nu$ data from the mass balance experiments of Figs. 27 through 36 vs the measured soots of the one outlyer (data from Fig. 32, JP8X-2429) this plot shows a much better correlation, and shows a tendency for the younger soots, from the 26 cm data, to lie closer to the abscissa. This is consistent with the interpretation of reduced optical constants for the young soots. Similarly, the "old" soots from the 66 cm data tend to lie below the extrapolation of the line through the 56 cm data, indicating the onset of agglomeration.

Molecular Weight Distribution of Fuel Components by FIMS

Experiments to determine molecular weight distributions in fuels and hydrocarbon pyrolysis products have been performed for AFR with a Field Ionization Mass Spectrometer (FIMS) at Stanford Research Institute. The technique was described by St. John et al. (26). FIMS is unique in its ability to produce unfragmented molecular ions from almost all classes of compounds.

Figure 56 shows the molecular weight distribution of collected PAH's as determined by FIMS for the 31 cm data of Fig. 35. A sample of soot and PAH's was collected at the exit of the entrained flow reactor after 31 cm in the reactor at 1300°C. The sample was heated in a probe in the FIMS from -50°C to 450°C. During this time 13% of the sample volatilized with the temperature dependence shown in Fig. 56b. The molecular weight distribution for all the volatile species is shown in Fig. 56c. The spectrum of acetylene pyrolysis products shows a very regular set of homologous series. This FIMS spectrum is inconsistent with simple formation of polyacetylenes (masses 170, 194, 218, 242, 266, etc.), since there are not peaks at these masses. These peaks are consistent, however, with the formation of PAH's. The maximum occurs at MW - 202 which is correct for pyrene and subsequent peaks are spaced by either 24 or 26 mass units. This pattern is consistent with successive additions of acetylene to the aromatic rings. Some possible structures are shown in Fig. 56a for the first few members of this series.

FIMS data for some of the butane pyrolysis soots and tars are shown in Fig. 57. Figure 57a is the soot (+ tar) scraped from the water-cooled extractor
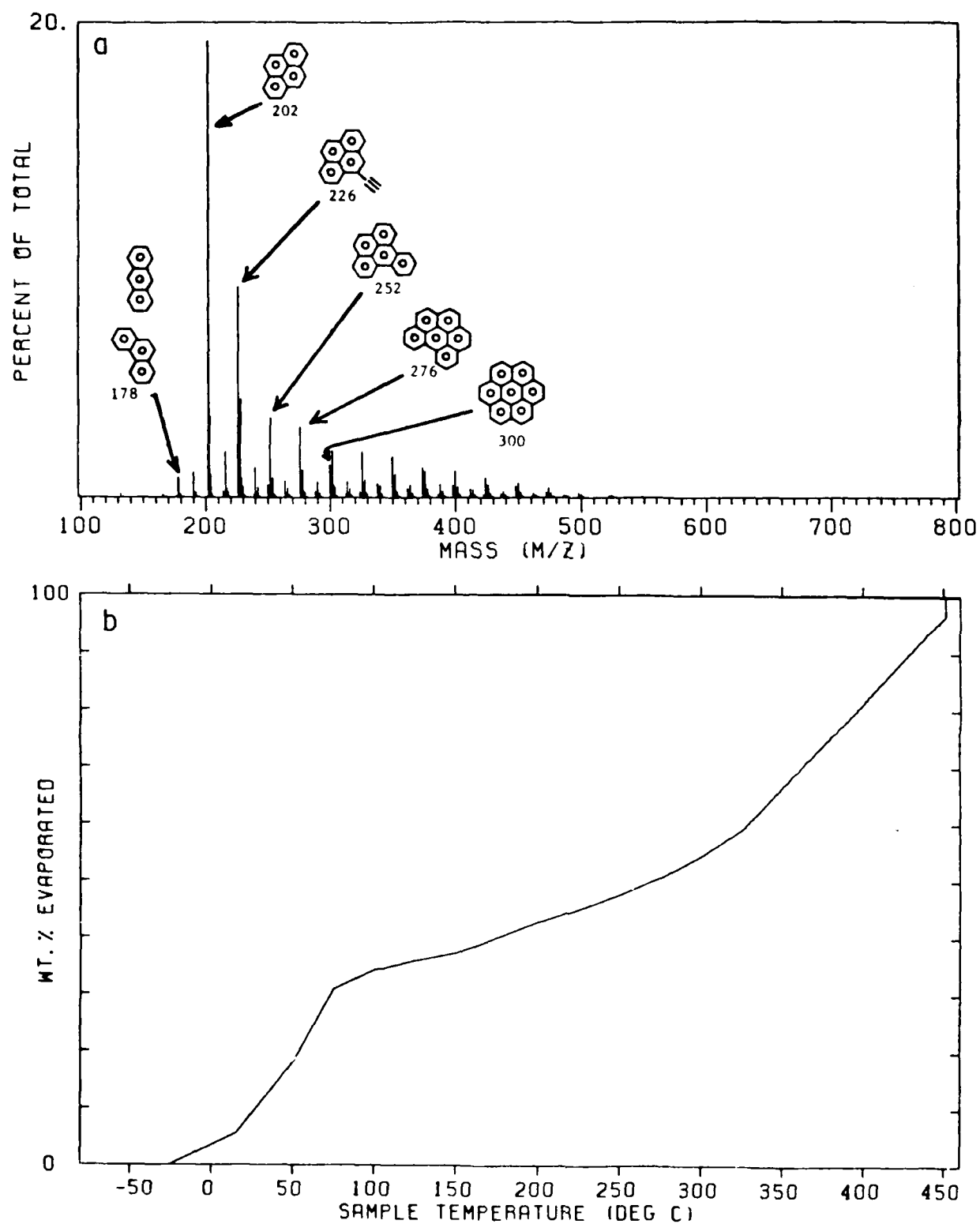
Figure 56. Molecular Weight Distribution for Products of Acetylene Pyrolysis. a) FIMS Spectrum, b) Temperature Dependent Weight Loss in Sample Probe.
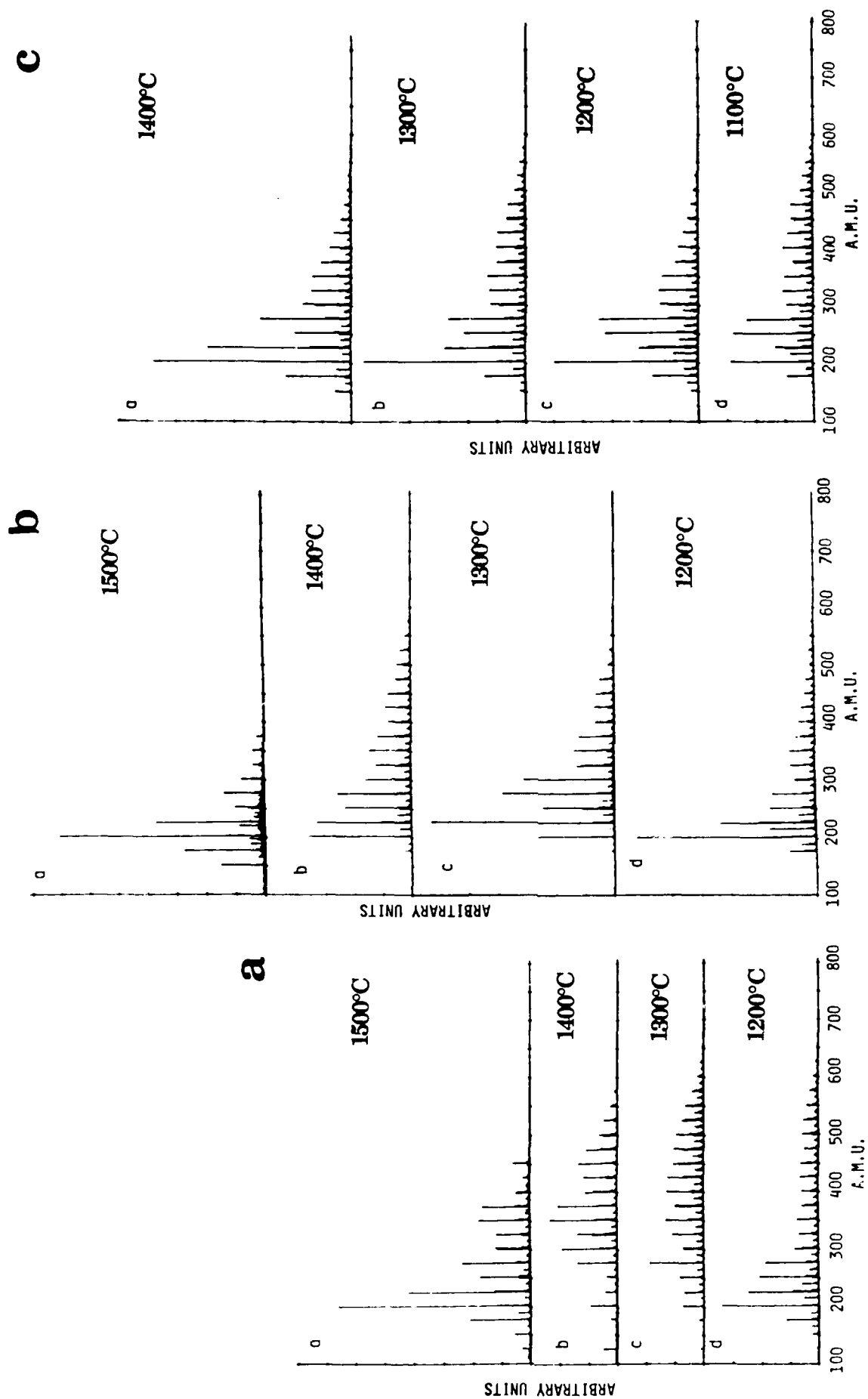
Figure 57. FIMS Spectra of a) Butane Soots Collected from Water-Cooled Extractor, b) Butane Soots Collected from Aluminum Foil Liner and c) Butane Tars Washed from Water-Cooled Extractor.

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located in the entrained flow reactor. Because of concerns that this soot was exposed to the hot gases with the extractor, an additional set of soot was taken from the aluminum foil liner in the gas collector. These are shown in Fig. 1b. Figure 57c shows the tars from the extractor (washed from the extractor with acetone, filtered and dried to remove the acetone). The spectra all look remarkably similar as a function of temperature. The locations of the vapor peaks, every 24 AMU, starting at 178 correspond to the sequence of 3, 4,... condensed aromatic rings.

TASK II - Fuel Characterization and Correlation

The objective of this task is to establish procedures for measuring the properties of fuel which affect combustion behavior using Fourier Transform IR spectroscopy as a diagnostic. This was done by measuring the infrared transmission spectrum for each of the liquid fuels, and developing correlations between the peaks in these spectra with the pyrolysis results of Task I, and with the literature data for the 25 NASA test fuels (20).

Experimental

FT-IR Liquid Cell Spectra - The fuels were characterized using FT-IR in the range from 400 cm^{-1} to 4000 cm^{-1}. In order to obtain quantitative spectra, two cells were used, one with a fixed, known pathlength, and a second with a variable pathlength cell. Example spectra are shown in Figs. 58a and b. All of the spectra are shown in Appendix B, Figs. B-1 through B-29. This double analysis was required because the fixed cell gives complete absorption on many of the peaks of interest as can be seen in the 2800-3000 cm^{-1} band in Fig. 56c. Therefore, the smaller peaks from the fixed cell such as the 1400 cm^{-1} peak in Fig. 58b were used to determine the pathlength, and thus calibrate the variable cell, which was adjusted until all peaks were on scale (Fig. 58b). The resulting spectra are then fit using an automated synthesis routine which resolves the spectra into a large number of Gaussian peaks (27). The position and width of these peaks are fixed at values which have been determined from analysis of a large number of liquid and solid spectra on model compounds (27-29). Only the height of these peaks are adjusted to fit the unknown spectrum. An example of the set of peaks used and the resulting fit to an unknown spectrum for coal is shown in Fig. 59. For liquids, the peaks were modified slightly to agree with literature interpretations (28,29). The fits

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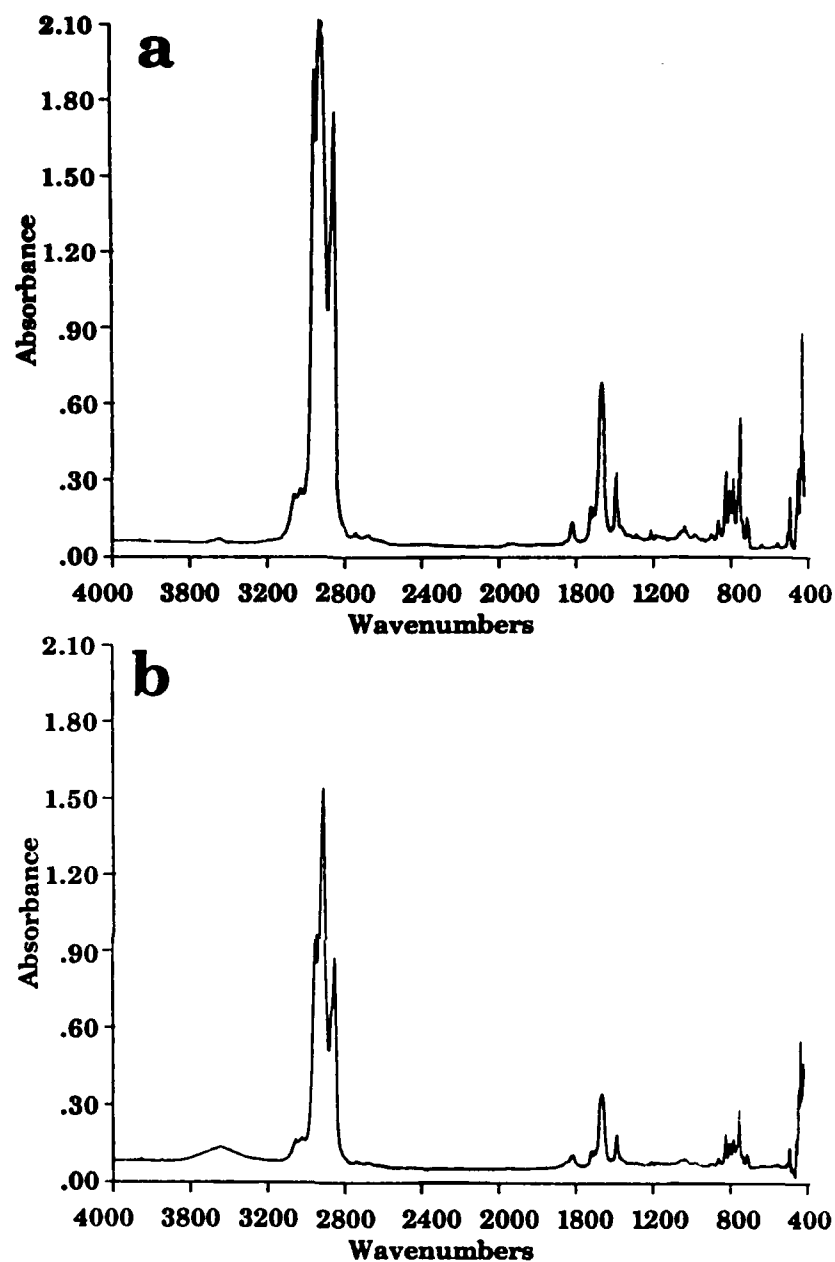
Figure 58. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel UTRC-2A.
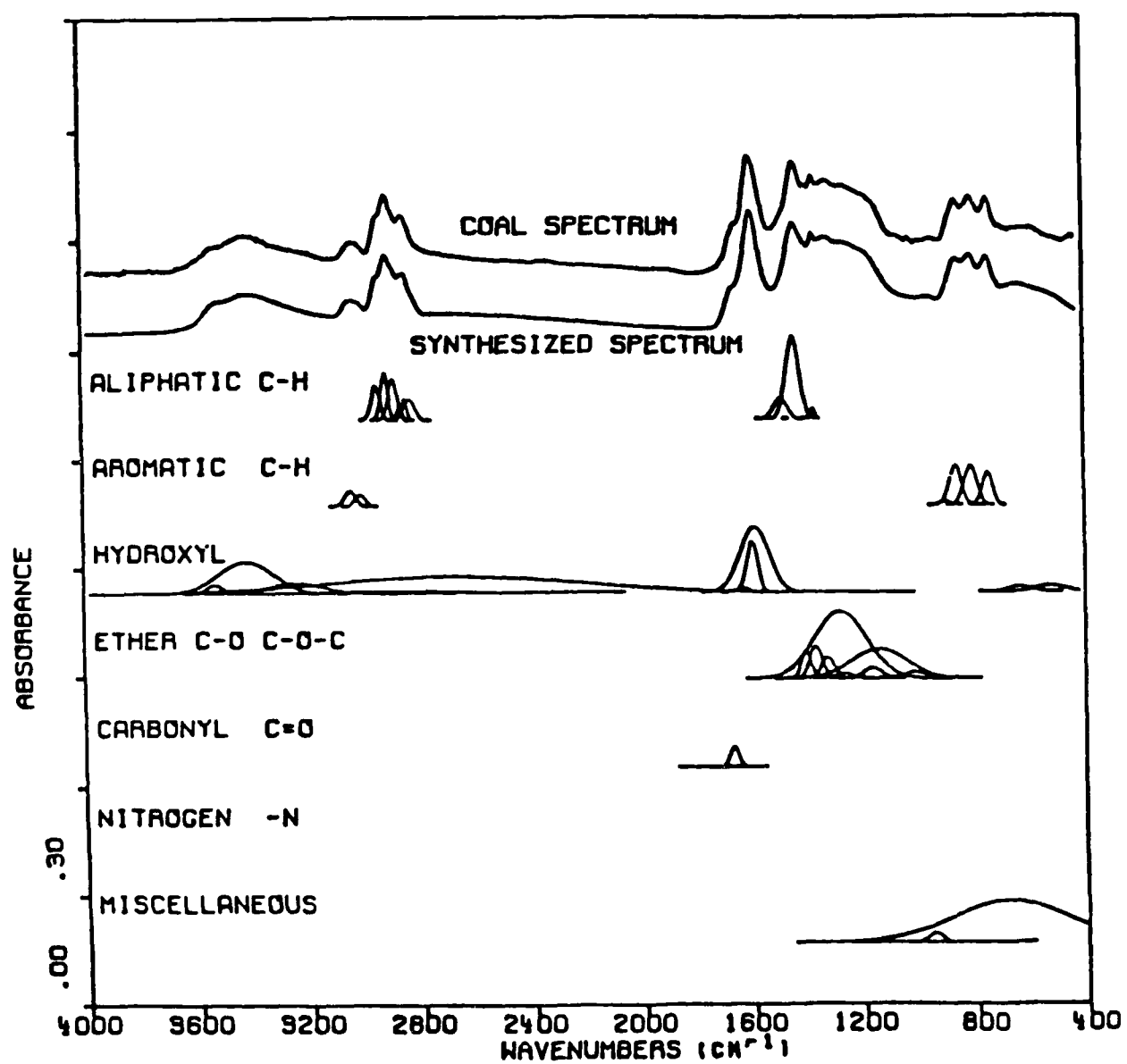
Figure 59. Synthesis of FT-IR Spectrum.

are usually better than 1%, which exceeds the experimental reproducibility of the spectrum ($\sim$5%). As indicated in Fig. 59, the peaks can be grouped into a few categories, (aromatics, aliphatics, etc.).

Entrained Flow Reactor Data - All of the fuels have been pyrolyzed at a fixed temperature and residence time (1573K and 700 ms) in AFR's entrained flow reactor (EFR) facility. This is a subset of the data taken in Task I. These conditions were chosen as a standard condition which provided partial conversion of the fuel to soot, and should provide a relative measure of the sooting potential of the fuels. The facility provides complete mass balances on the pyrolysis products including soot (all insoluble solids), tar (solids soluble in dichloromethane) and gases (CH_4, C_2H_2, C_2H_4, C_2H_6, C_3H_6, heavy olefins, etc., by FT- IR; and H_2, benzene by gas chromatography). In order to minimize the effects of fuel vaporization and reduce the heat load on the reactor, a heated fuel injector was used. This injector was maintained at 250°C, which is sufficient to fully vaporize some of the fuels, and should partially vaporize all the fuels. Thus we expect that all of the fuels were pyrolyzed at similar conditions.

Data Sets - The data set for the fuel correlations consists of three groups. The first group is the FT- IR liquid cell spectra which have been reduced to a set of 51 Gaussian peaks, which reproduce the original spectra to better than the experimental reproducibility. These data are used in a factor analysis in either of two ways in this discussion: 1) The peaks are grouped into functional categories such as methyls, carboxyls, aromatics, etc., to generate factors, or 2) The peaks are used individually to generate factors.

The second set of data is the pyrolysis results at 1300°C, which includes a full product slate of soot, tar, H_2, CH_4, C_2H_2, C_2H_4, C_2H_6, C_3's and benzene. These are treated as dependent variables, dependent on the factors generated from the liquid cell spectra.

The third set of data is that of Rosfjord (20) at UTRC. Most of the fuels were originally formulated and characterized in a UTRC-NASA program for use in a combustion test facility. His data includes 66 measurements of physical and chemical properties and combustion results.

Factor Analysis

The purpose of factor analysis is to find an underlying small set of common factors which can explain a large number of measurements. For example, in fuels

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with a wide range of chemical compositions, one might hope to find that the sooting behavior could be explained by a single determining factor, such as aromatic content, or the difference between aromatic content and hydrogen content. Factor analysis is the process of doing this, and includes both physical intuition and mathematical methods.

Details of Method of Correlating FT-IR Spectra with Other Properties of Jet Fuels

The starting point of the mathematical factor analysis is a set of peak areas obtained using the fitting procedure described above. The peak deconvolution algorithm was developed previously at AFR. For the specific example of the jet fuels, there are 51 peaks used in each fuel spectrum. The peak areas for two fuels are listed in Table 3. The basic technique for the factor analysis is the principal components method of Hotelling, and is described in Chapter 8 of Ref. 30.

The first step is to compute all the pairwise correlations (r_{ij}) between the peaks.

$$ r_{ij} = \frac{\sum_{n=1}^{nfuel} (x_{hi}-\langle x_i \rangle)(x_{hj}-\langle x_j \rangle)}{(nfuel-1) \cdot s_i \cdot s_j} \tag{8} $$

where

x_{hi} is the ith peak area for the hth fuel

$\langle x_i \rangle = \sum_{h=1}^{nfuel} x_{hi}/nfuel$ is the sample mean area of the ith peak

$s_i^2 = \sum_{h=1}^{nfuel} (x_{hi}-\langle x_h \rangle)^2/(nfuel-1)$ is the sample variance in the area of the hth peak

This correlation matrix (51x51 for the case of 51 peaks), together with the means $\langle x_i \rangle$ and the variances s_i^2 are all the information needed for the analysis.

The next step is to find the factors which best describe the correlations. Mathematically, (see Ref. 30) this consists of solving the eigenvalue problem:

TABLE 3

Peak Areas (abs.cm-1) for two fuels.

(This table is split to indicate the functional groups)

Fuel DF2 (high soot)

57.7400	6.9320	39.5500	7.8100	33.6300	18.2300	3.7810	0.7152	(aliphatics)
0.0000	0.6314	23.4100	0.2875	4.1010	0.0000	0.2103	0.8746	
3.7990	1.3200	0.3383	0.4821	0.8232	1.9850	0.0203		(aromatics)
30.1400	0.0000	2.7580	1.6310	0.4545	1.8310	10.3900	1.5360	(-OH)
0.8450	2.0020						4.2820	
0.0000	1.8620	0.9921	3.8390	0.2657	5.4040	1.1680	0.9292	(C-O)
	1.4400	1.4400						
			0.2432	0.4701	0.0896	0.5787		(C=O)
2.4370	0.0183						7.3490	(Miscellaneous)
	0.6847							

Fuel JP8-X 2949 (low soot)

87.2500	11.0400	37.6400	6.3020	47.8000	18.6700	3.2870	0.7996	(aliphatics)
0.0000	0.0000	36.7900	1.5910	0.0000	0.0000	0.3035	0.7485	
2.4410	0.9076	0.7497	0.6123	0.3754	0.3400	0.0000	0.0000	(aromatics)
1.2310	17.6200	0.1860	4.4590	0.0000	0.0000	0.0000	0.9141	(-OH)
1.3780	0.0000	0.9377	0.7031	0.0000	6.3260	2.0700	0.0000	(C-O)
0.1107	2.4300	2.1030	0.0000	0.1994	0.0000	0.0000	0.0000	(C=O)
4.4840	0.0000	0.0000					4.0360	(Miscellaneous)

$$\sum_{j=1}^{npeak} r_{ij} a_{kj} = \lambda_k \cdot a_{ki} \tag{9}$$

for the eigenvectors a_k, and their eigenvalues, λ_k.

There are npeak such eigenvalues and eigenvectors, each eigenvector having npeak components. This procedure is equivalent to rotating a 51 dimensional coordinate system so that most of the variance in the data lies along the axes of the new coordinate system. The new coordinate axis containing the maximum variance has components or projections on each of the original coordinates (peak areas), and thus represents the single linear combination of peak areas which best fits the data. An example in two dimensions can help explain this. Consider the data in Fig. 60. The means and variances are indicated on the axes x_1 and x_2.

For the data in the figure, the correlation $r_{12} = 1.0$.
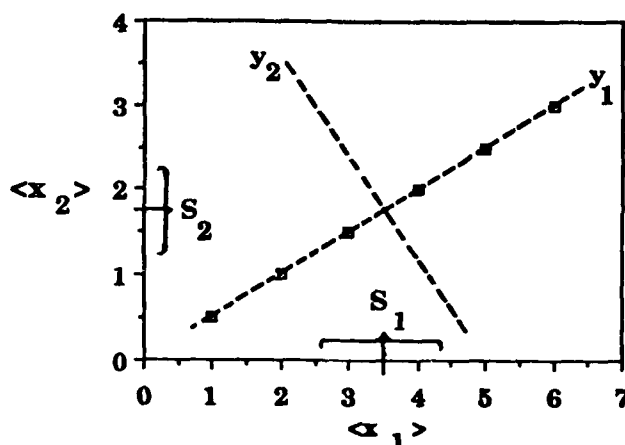
Fig. 60. Example of Correlated Measurements in Two-Dimensions.

By changing to a new coordinate system, shown as (y_1, y_2), the data all lie on the y_1 axis, the correlation between y_1 and y_2 is zero, and the equation of axis y_1 in terms of x_1 and x_2 is the linear combination that best explains the data. All of the variance in x_1 and x_2 is now contained in y_1.

The variances in the new coordinate system are given by the eigenvalues, while the axes of the new system are the corresponding eigenvectors. Just as in the two dimensional example above, where one of the vectors (y_2) can be discarded as containing no information about our original data (x_1, x_2), so too in the case of our 51 peaks and factors in the fuels case. The resulting factors (eigenvectors) and sample variances (eigenvalues) are shown in Table 4 for the first 8 factors. The fraction of the total variance explained by each eigenvector is given by $\lambda_k/npeak$ (see Ref. 1). Thus, by adding up the first 8 eigenvalues, we see that

TABLE 4

Factors based on 24 fuels, with eigenvalues.

Factor #   1 Eigenvalue = 12.716800

0.7051	0.3671	0.5732	0.4166	0.8677	0.7800	0.4565	-0.9227
0.2454	0.3517	0.7611	-0.7779	-0.0095	-0.2226	-0.4170	-0.6826
-0.8686	-0.9149	-0.6557	-0.9423	-0.4597	-0.5373	-0.0165	0.3651
0.3670	0.0859	0.5016	-0.6134	0.1226	0.2530	0.3966	0.3682
-0.9260	0.4427	-0.6412	0.2798	-0.0978	-0.0136	0.0439	0.2295
-0.0816	-0.5462	0.1765	0.0166	-0.0162	0.5098	-0.0389	0.1082
-0.1252	-0.0873	0.4224					

Factor #   2 Eigenvalue = 9.801150

0.2883	0.6058	0.2382	0.2278	0.3650	0.1069	0.4603	-0.2458
-0.2841	-0.2298	0.2158	-0.0185	-0.4197	-0.3372	0.4682	-0.1152
-0.1719	-0.2008	-0.1445	-0.1364	-0.2202	-0.2754	-0.0991	-0.7891
-0.7429	0.6878	-0.7049	-0.0554	0.3690	-0.3761	-0.5340	-0.8275
-0.0969	-0.7218	0.0126	-0.7050	-0.0663	-0.4638	0.5398	-0.4705
0.1623	-0.0584	0.5345	-0.4548	-0.8519	-0.5500	-0.7358	-0.6546
-0.0045	0.0906	-0.4421					

Factor #   3 Eigenvalue = 6.251490

-0.2787	-0.4181	0.6633	0.7530	0.0185	0.4871	0.5937	-0.0129
0.2019	0.4087	-0.2922	0.3031	0.5542	-0.7485	0.4074	-0.4166
0.2567	0.1829	-0.4571	-0.0139	-0.1077	0.4573	0.5755	-0.1157
-0.1281	-0.2128	0.0055	-0.0516	-0.1172	-0.6716	0.0848	-0.2117
0.2204	-0.1050	-0.2639	-0.0722	-0.0600	0.0372	-0.2005	0.5290
-0.0917	0.2631	-0.5514	-0.3228	0.0757	-0.2422	0.2278	0.2991
-0.2542	-0.0082	-0.3730					

Factor #   4 Eigenvalue = 5.140550

0.2018	-0.2505	-0.1451	-0.2435	0.1590	0.1846	0.1262	-0.1820
-0.4501	0.0956	0.3404	0.2605	-0.2717	-0.3238	0.2278	-0.4393
-0.1673	0.2483	-0.4703	0.2023	0.5078	0.3528	-0.0054	0.2383
0.2947	0.1007	0.0115	0.0106	0.2432	0.1957	0.0085	0.1866
0.2231	0.3113	0.4599	-0.4674	0.4800	0.3121	0.4990	-0.3387
0.3730	0.5575	0.5446	-0.4702	0.3294	0.0243	0.2084	0.2239
-0.6046	0.2155	0.3980					

TABLE 4 (concluded)

Factor #   5   Eigenvalue = 4.168080
```
 -0.0590   -0.3315   -0.1408   -0.2677   -0.0452   -0.0405   -0.2826   -0.0379
 -0.2514    0.3743    0.1319    0.0274    0.1921    0.1488   -0.2341   -0.0148
 -0.0007    0.0287    0.0323   -0.1065    0.0081    0.3474    0.5890   -0.1830
 -0.1058   -0.3079   -0.4327   -0.2002   -0.4957    0.4470    0.4434   -0.1444
 -0.0040   -0.1196   -0.3890   -0.1094    0.1380   -0.5976   -0.2361   -0.1266
 -0.0872   -0.3009   -0.1711   -0.4107   -0.0850    0.0704   -0.4145   -0.5327
 -0.5884    0.2941    0.4581
```

Factor #   6   Eigenvalue = 2.924650
```
  0.0206    0.0288    0.2268    0.0912   -0.2333   -0.0261    0.1582   -0.1042
 -0.5190    0.5014    0.0439   -0.2628   -0.4221   -0.2421    0.2224    0.2647
 -0.0564   -0.0836    0.0342    0.0408    0.2776    0.0555    0.0593    0.2498
  0.3375   -0.3330    0.0605    0.5432    0.0561   -0.1155   -0.4763    0.0948
 -0.1063    0.3206   -0.0315    0.2091   -0.0257   -0.3078   -0.2544   -0.4092
 -0.2549   -0.3162   -0.0853    0.1075   -0.1475   -0.2600   -0.0474    0.0459
  0.0287    0.3121   -0.1661
```

Factor #   7   Eigenvalue = 2.755080
```
 -0.2520    0.0782    0.1476    0.1249   -0.0845   -0.1736    0.0552   -0.0977
  0.2665    0.1953   -0.2558   -0.1800   -0.1928   -0.1337   -0.4457    0.1454
 -0.2465    0.0066    0.1348    0.0311    0.0312    0.2915    0.0243   -0.1064
 -0.0782   -0.1500    0.0381    0.2354    0.0101    0.0136    0.1579   -0.0397
 -0.1301   -0.0837   -0.1660   -0.2681    0.7950    0.2552    0.4693    0.3179
  0.4813   -0.3232    0.0132    0.2565   -0.1869   -0.1179    0.1715   -0.0700
  0.1762    0.4101    0.0006
```

Factor #   8   Eigenvalue = 1.986950
```
  0.3950    0.1415   -0.0502   -0.0630    0.0422    0.1028   -0.2195    0.1156
 -0.3524    0.2188    0.2033    0.1052    0.1216    0.0812   -0.0667    0.0480
  0.0894   -0.0115    0.2306   -0.0858   -0.4132    0.0520    0.4465   -0.0104
  0.0071    0.1048    0.1502    0.3586   -0.0980    0.0449   -0.1461    0.0173
 -0.0273   -0.0857   -0.2549   -0.0014    0.1091    0.1621    0.0912   -0.0611
  0.4754    0.0322   -0.0873   -0.0656    0.0940   -0.3162    0.0040    0.2659
  0.0733   -0.5413   -0.0267
```

these 8 factors explain 90% of the data. The order of the peaks in the factors is the same as in Table 3.

It is usually not possible to draw any conclusions from looking at the factors directly, but they are useful in correlating the data with other measurements. This is because we have now concentrated the variance in the data into a few (8 or 9) factors, whereas in the original data it was spread out over 51 spectral peaks.

The next step in the procedure is to correlate parameters of interest such as the soot measurements from the spectra using these factors. To do this we compute the projection of each fuel spectrum onto the 8 factors to obtain the contribution of each factor (f_k) to the specific fuel; and then do a least-squares fit of the soot measurement with these projections as follows:

Form projections p_{hk}:

$$p_{hk} = \sum_{j=1}^{npeak} x_{hj} \cdot f_{kj}/s_j \qquad\qquad \begin{array}{l} h = 1, nfuel \\ k = 1, nfactor \end{array} \qquad (10)$$

$$= \text{contribution of } k^{th} \text{ factor to } h^{th} \text{ fuel.}$$

Compute linear regression between y_h (eg. soot) and p_{hk}

$$y_h = s_y \sum_{k=1}^{nfactor} b_k \cdot p_{hk} \qquad\qquad (11)$$

where

s_y^2 is sample variance of y_i

b_k are regression coefficients

Choose b_k, such that

$$\sum_{h=1}^{nfuel} [y_h(\text{computed}) - y_h(\text{measured})]^2 \text{ is minimized.} \qquad (12)$$

The minimization reduces to a set of nfactors simultaneous linear equations in b_k.

For each k:

$$\sum_{h=1}^{nfuel} \sum_{k'=1}^{nfactor} b_{k'} \cdot P_{hk} \cdot P_{hk'} = \sum_{h=1}^{nfuel} y_h \cdot P_{hk} \qquad (13)$$

As an example, the b_k's for the soot regressions are shown in Table 5. In addition, in Table 5 are shown the contributions c_j of each peak to these fits.

$$c_j = \sum_{k=1}^{nfactor} s_y \cdot b_k \cdot f_{kj}$$

These c_j are the regressions of the y_i with the original peaks, as can be seen by combining Equations (3) and (4).

$$y_h = s_y \cdot \sum_{k=1}^{nfactor} b_k \cdot \left[\sum_{j=1}^{npeak} x_{hj} \cdot f_{kj}/s_j \right]$$

$$= \sum_{j=1}^{npeak} \left[\sum_{k=1}^{nfactor} s_y \cdot b_k \cdot f_{kj} \right] \cdot x_{hj}/s_j = \sum_{j=1}^{npeak} c_j \cdot x_{hj}/s_j \qquad (14)$$

The final step is to compute the correlation of the calculated soot with the actual soot.

$$r = \frac{\sum\limits_{h=1}^{nfuel} (y_h(computed) - \langle y(computed) \rangle)(y_h - \langle y \rangle)}{(nfuel-1) \cdot s_y(computed) \cdot s_y} \qquad (15)$$

Results

From experience we expect that the liquid cell FT-IR spectra completely define the liquid, and that the pyrolysis and combustion data can be predicted from this. Thus we have generated the factor matrix from the FT-IR spectra only. Second, since we expect that the functional groups in the fuel (e.g. methyl) and not the individual peaks in the spectrum are the important feature, we look for ways of grouping all the peaks according to the functional group which causes them.

The mathematical part of factor analysis consists of finding those linear

TABLE 5

Regression Coefficients

b(0)	b(1)	b(2)	b(3)	b(4)	b(5)	b(6)	b(7)	b(8)
52.951610	-0.276940	0.056628	-0.217369	-0.019662	-0.139711	0.239600	-0.245557	0.001835

Contribution of each peak to fit,   c(j)

-0.0466	0.0627	-0.2489	-0.2329	-0.2555	-0.2773	-0.1685	0.2525
-0.2744	-0.1808	-0.0864	0.1210	-0.2167	0.1658	0.2443	0.3116
0.2256	0.1717	0.2530	0.2691	0.1852	-0.0799	-0.1993	-0.0138
-0.0068	0.0597	-0.1144	0.2787	0.0877	-0.0426	-0.3738	-0.0538
0.2056	-0.0328	0.3137	0.0387	-0.1935	-0.0894	-0.0909	-0.3571
-0.1218	0.1255	0.0906	0.0691	-0.0441	-0.1639	-0.0801	-0.0334
0.1475	-0.0412	-0.1728					

combinations of the data (eigenvectors) such that the correlations between the eigenvectors is zero, together with a measure of the significance of the eigenvectors (eigenvalue). As an example, if we had a set of 50 fuels which were made up of different mixtures of say, benzene and hexane, we might find that two of the vectors would have non-zero eigenvalues (significance) one of which contained the IR peaks for hexane, the other would have all the benzene peaks, and the remaining 48 eigenvectors would have zero significance. In this case we would have two factors which are identifiable as chemicals. In practice we are apt to find that one of the factors is, for example, a weighted sum of the spectra, and the other is the weighted difference between the spectra, making interpretation of the factors difficult.

In our case we find that all the FT-IR data can be explained to within experimental error with a few (8 or 9) factors, whereas we started with 51 peaks. To obtain predictors of the pyrolysis and combustion results we do least square regressions between the factors and the dependent variables (Figs. 61a-f). With these fits we obtain correlations between the predictions and the data of $r^2 > 0.80$ and usually better than 0.9. Not surprisingly, the correlation between the IR factors and Rosfjord's chemical characterization data is excellent (H_{total}, saturated hydrocarbons, total aromatics). This verifies our assumption that the factors define the fuel chemical composition. Of more interest is the correlation of the IR factors with the pyrolysis products at 1300°C, and with Rosfjord's combustion data. The best fit is to Rosfjord's dome radiation (Fig. 61a and 61b). Dome radiation is the total hemispherical radiant heat load to the inlet dome of the combustor. This radiation value is a measure of the amount of soot in the region of the radiation detector since the soot is the major contributor to the radiant energy. The agreement between the soot predicted from the chemical data as measured by FT-IR and soot as measured by radiation in a combustor is excellent. A second measure of the soot is the smoke number (20). This correlation is shown in Fig. 61b.

The fits to the major pyrolysis products at 1300°C and 700 ms residence time are shown in Figs. 61c and 61f. The trends are clear, and agree with Rosfjord's data. This time-temperature regime was chosen to provide survey of partial pyrolysis of the fuel for use in kinetics modeling and as such, may not provide a measurement of the maximum sooting behavior of the fuel. Some of these products can be classed roughly as final products of the pyrolysis process (soot, CH_4, polyacetylenes, PAH's) which react to form the final products. As a result, the fit to the soot is better than that for the acetylene.
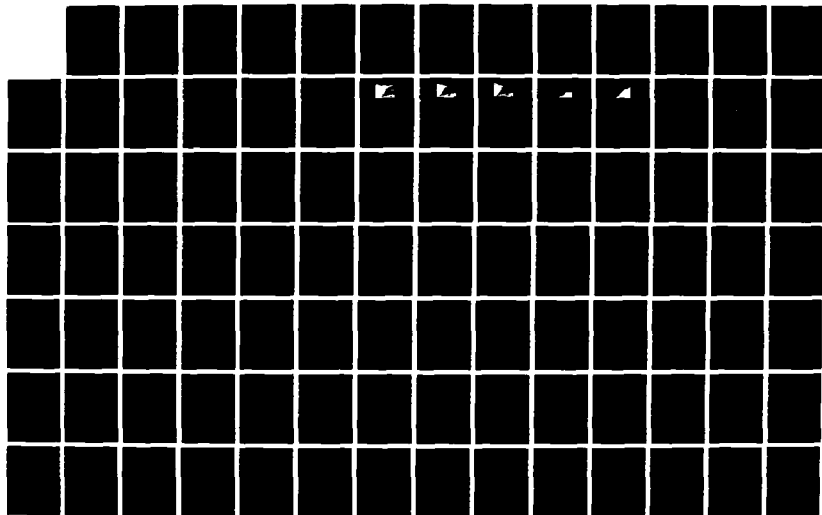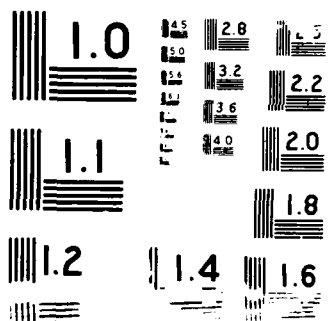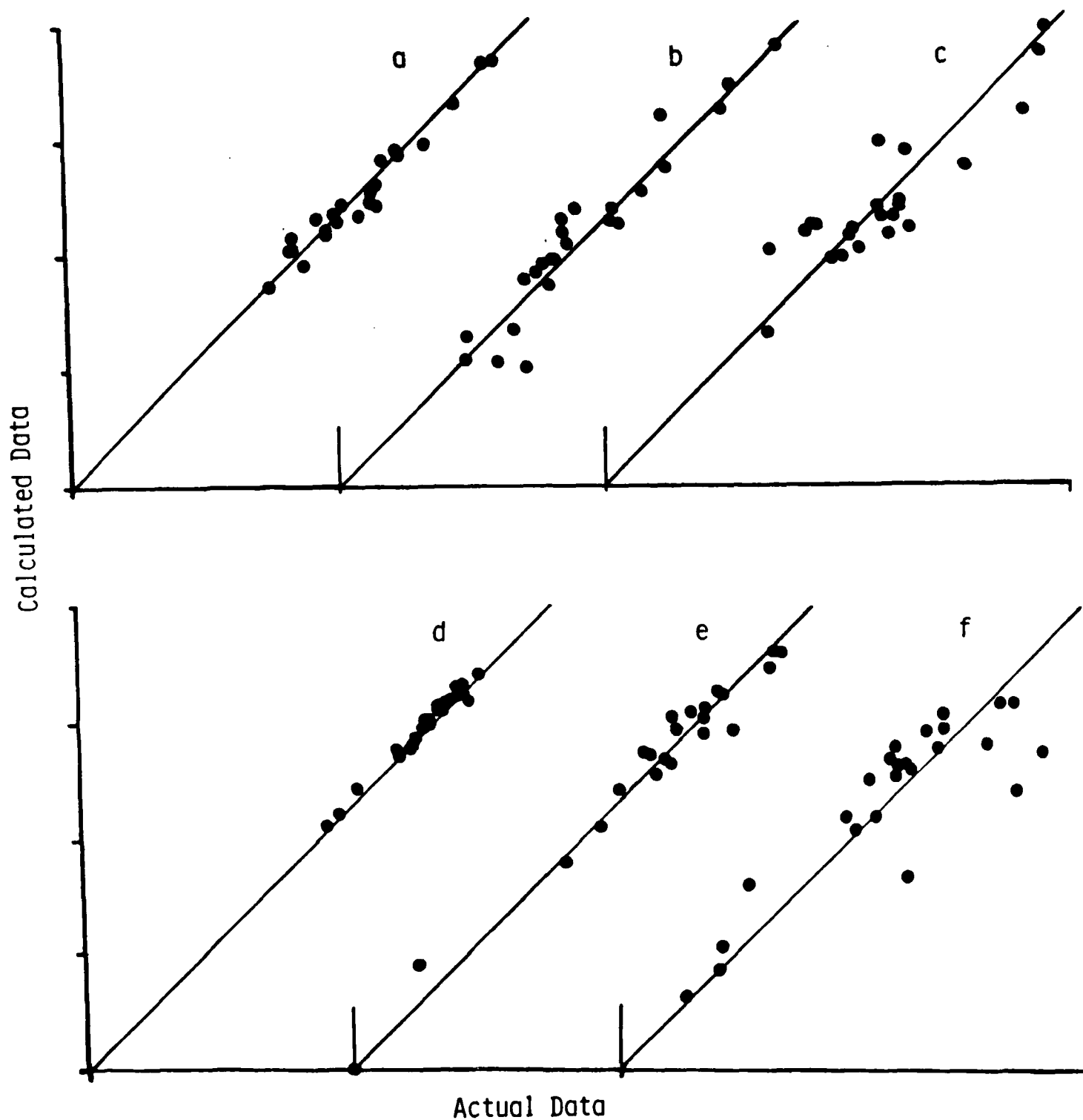
Figure 61. Correlations Plots Between Actual and Predicted Results for Six Fuel Parameters, a) Combustor Dome Radiation, b) Smoke Number in Combustion, c) Soot from Entrained Flow Reactor, d) Total Hydrogen, e) H/C Ratio and f) Acetylene from Entrained Flow Reactors. Scales are Arbitrary with Offset Origins, Lines are 45° Parity Lines.

Given the clear correlation between sooting behavior of the fuels and the structural details of the fuels as determined by FT-IR, we can now look at the structural features which give rise to, or which inhibit sooting. This is done by calculating the importance of the FT-IR peaks in the regression to the regression data. In an attempt to gain some physical understanding of these regressions, we have gone back to the original data and grouped the peaks together in what should be reasonable groups. Six groups were chosen consisting of the following peaks:

Group 1	peaks 1,5,11	$R-CH_2-R$
Group 2	peaks 3,4,7	$R-CH_3$
Group 3	peak 6	$-R-R-$
Group 4	peak 13	$-CH_2-$
Group 5	peaks 17,18	Aromatic stretch
Group 6	peaks 19,20,21,22	Aromatic wag
Group 7	all other peaks	

To estimate the significance of each of these groupings, the peak contributions from Table 5 were added algebraically within the above groups and normalized by the algebraic sum of all the peaks. The results of this computation together with the fit correlations are shown in Table 6 for several measured parameters. These groupings help provide an understanding of the correlation between the actual infrared spectra and various measured properties of the fuel. The sign of the entry in Table 6 indicates the direction of the effect, and the amount of the entry is the magnitude of the effect. As an example, the soot items (dome radiation, smoke number and soot (EFR)) all are strongly depressed by the first three columns in Table 6 which represent β-hydrogens. In contrast, the total hydrogen is positively correlated with the β-hydrogen, as expected.

The groups selected for Table 6 are only those which gave major contributions to all the dependent variables. The balance of the information is spread among the remaining peaks as indicated by the column labeled "other".

The results indicate that all fuels have an "intrinsic" sooting potential which is strongly depressed by aliphatic hydrogen in locations which make it readily available for capping of radicals (i.e. α and β - to the aromatic rings). The presence of aromatic structures only weakly increases the sooting potential (compared to the strong decreasing effect of the aliphatics).

TABLE 6

INFLUENCE OF STRUCTURAL FEATURES ON MEASUREMENTS
(fractional peak areas)

	Corr.r	R-CH$_2$R	R-CH$_3$	-R-R-	CH$_2$-	Ar Stretch	Ar Wag	Other
Soot (EFR)	0.890	-15	-24	-10	-8	15	24	-4
C$_2$H$_2$ (EFR)	0.854	20	15	8	3	-9	-24	20
Dome Radiation	0.979	-11	-16	-7	-6	7	18	35
Smoke Number	0.958	-9	-14	-7	-8	9	16	37
H$_{total}$	0.990	10	19	7	4	-9	-17	-34
Aromatics	0.981	-19	-20	-9	-1	16	21	16
Saturated H/C	0.984	20	17	8	1	-15	-21	-18
Density	0.968	-4	-24	-9	-9	0	12	41
Flash Point	0.682	16	1	2	0	-13	-17	-51
Freeze Pt	0.752	4	-32	-6	-14	-7	16	20
Olefins	0.612	3	12	-4	-7	-6	0	72
Paraffins	0.962	-10	30	5	5	-5	-7	-39
Smoke Point (mm)	0.916	5	13	6	9	-8	-20	-41
Viscosity	0.918	-16	-15	-14	-9	-12	-3	30

Conclusion

The results of this study show that the characterization of the liquid fuels by FT- IR spectra can be concisely summarized by a few factors which can reproduce the spectra to within experimental error. Secondly, these factors can be used to predict the combustion properties of the fuels, in particular the sooting behavior. Third, the regressions used to predict soot can be used to determine structural functional groups which are important for sooting behavior.

Task III - Drop Vaporization Studies - (deleted from original contract).

Task IV - Modeling

The objective of this task was to develop models to correlate combustion behavior with fuel properties. Progress was made in three areas. The hydrocarbon cracking model began in Phase I was extended using a modified Rice-Kossiakoff-Herzfeld (RKH) mechanism. This model predicts the decomposition of long chain aliphatics into small molecules, (C_2H_2, C_2H_4, H_2). Secondly, a soot model based on published free radical mechanisms and rates (23 and refs. therein) was implemented on our minicomputers and used to predict the growth of the soot precursors from the small molecules produced. Third, a heat transfer model was developed to provide the temperature-time profiles required by both models.

Examining the data of Task I, for the simple hydrocarbons, as well as for the jet fuels, shows that all the fuels appear to crack down to these small species. Thus the modeling approach has been to combine the hydrocarbon cracking model, which can treat large "generic" hydrocarbons, with the soot submodel which uses specific small chemical species. The comparison between models and experiment look very encouraging. In this section we discuss the two models, together with the heat transfer model and comparison with the pyrolysis measurements of Task I.

Hydrocarbon Cracking Model

As a result of the combined Phase I and Phase II SBIR programs, a kinetic model for the pyrolysis of complex mixtures of hydrocarbons was developed. This free radical model uses conventional elementary reaction steps and rate constants taken from the literature. It was extensively validated using both in-house and literature data. The reactions which have been included, their rate constants, and literature references (31,32) are listed in Table 7.

The model makes predictions for the concentrations of H_2, alkanes, 1-alkenes,

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TABLE 7 - Hydrocarbon Cracking Model, $k = AT^n \exp(-E/RT)$.

	$\log_{10}A$ (1, moles, sec)	n	E (kcal/mole)	REF
INITIATION:				
1. $C_2H_6 \longrightarrow CH_3 + CH_3$	19.35	-1.0	88.3	a
2. $C_3H_8 \longrightarrow CH_3 + C_2H_5$	16.9	0.0	85.1	b
3. $C_4H_{10} \longrightarrow CH_3 + C_3H_7$	17.5	0.0	85.7	b
4. $RCH_3 \longrightarrow R + CH_3$	16.8	0.0	85.4	b
5. $C_4H_{10} \longrightarrow C_2H_5 + C_2H_5$	16.4	0.0	82.1	b
6. $RC_2H_5 \longrightarrow R + C_2H_5$	16.8	0.0	81.9	b
TERMINATION:				
7. $R + R' \longrightarrow RR'$	9.8	0.0	0.0	Text
DECOMPOSITION:				
8. $C_2H_5 + M \longrightarrow C_2H_4 + M + H$	12.3	0.0	30.0	a
9. $2-C_3H_7 \longrightarrow C_3H_6 + H$	13.9	0.0	40.4	b
10. $1-C_3H_7 \longrightarrow C_3H_6 + H$	13.2	0.0	38.6	b
11. $1-C_3H_7 \longrightarrow C_2H_4 + CH_3$	13.1	0.0	32.5	b
12. $C_2H_3 + M \longrightarrow C_2H_2 + M + H$	11.9	0.0	31.5	a
13. $Y_{1,3}PR_1 \longrightarrow Y_{1,3}O_{1-1} + Y_{1,3}CH_3, \, i>4$	13.9	0.0	33.0	b
14. $Y_{1,1-2}PR_1 \longrightarrow Y_{1,1-2}O_{1-1} + Y_{1,1-2}CH_3, \, i>4$	13.9	0.0	33.0	b
15. $Y_{1,4}PR_1 \longrightarrow Y_{1,4}O_{1-2} + Y_{1,4}C_2H_5, \, i>4$	12.7	0.0	29.1	b
16. $Y_{1,1-3}PR_1 \longrightarrow Y_{1,1-3}O_{1-2} + Y_{1,1-3}C_2H_5, \, i>4$	12.7	0.0	29.1	b
17. $Y_{1,j+2}PR_1 \longrightarrow Y_{1,j+2}O_{1-j} + Y_{1,j+2}PR_j, \, i>5; \, j=3,1-2$	13.4	0.0	28.8	b
18. $Y_{1,1-j-1}PR_1 \longrightarrow Y_{1,1-j-1}O_{1-j} + Y_{1,1-1-1}PR_1, \, i>5; \, j=3,1-2$	13.4	0.0	28.8	b
19. $Z_{1,1-2}OR_1 \longrightarrow Z_{1,1-2}D_{1-1} + Z_{1,1-2}CH_3, \, i>5$	13.9	0.0	33.0	b
20. $Z_{1,1-3}OR_1 \longrightarrow Z_{1,1-3}D_{1-2} + Z_{1,1-3}C_2H_5, \, i>6$	12.7	0.0	29.1	b
21. $Z_{1,1-j-1}PR_1 \longrightarrow Z_{1,1-j-1}D_{1-j} + Z_{1,1-j-1}OR_j, \, i>7; \, j=3,1-4$	13.4	0.0	28.8	b
22. $Z_{1,j+2}OR_1 \longrightarrow Z_{1,j+2}O_{1-j} + Z_{1,j+2}OR_j, \, i>5; \, j=3,1-2$	13.4	0.0	28.8	b
H TRANSFERS:				
23. $H + CH_4 \longrightarrow H_2 + CH_3$	11.0	0.0	11.9	a
24. $H + C_2H_6 \longrightarrow H_2 + C_2H_5$	-.27	3.5	5.2	a
25. $H + C_3H_8 \longrightarrow H_2 + C_3H_7$	10.8	0.0	7.7	b
26. $H + C_2H_4 \longrightarrow H_2 + C_2H_3$	4.18	2.0	6.0	a
27. $H + C_3H_6 \longrightarrow H_2 + C_3H_5$	11.0	0.0	3.5	b
28. $H + RH \longrightarrow H_2 + R$	11.1	0.0	7.7	b
29. $CH_3 + H_2 \longrightarrow CH_4 + H$	9.68	0.0	11.43	a
30. $CH_3 + C_2H_6 \longrightarrow CH_4 + C_2H_5$	-3.26	4.0	8.28	a
31. $CH_3 + C_3H_8 \longrightarrow CH_4 + C_3H_7$	8.8	0.0	10.5	b
32. $CH_3 + C_3H_6 \longrightarrow CH_4 + C_3H_5$	8.2	0.0	8.8	b
33. $CH_3 + RH \longrightarrow CH_4 + R$	8.6	0.0	9.6	b
34. $C_2H_5 + H_2 \longrightarrow C_2H_6 + H$	-.01	3.5	27.32	a
35. $C_2H_5 + CH_4 \longrightarrow C_2H_6 + CH_3$	7.48	0.0	12.5	a
36. $C_2H_5 + C_3H_8 \longrightarrow C_2H_6 + C_3H_7$	7.7	0.0	10.4	b
37. $C_2H_5 + C_3H_6 \longrightarrow C_2H_6 + C_3H_5$	8.0	0.0	9.8	b
38. $C_2H_5 + RH \longrightarrow C_2H_6 + R$	8.0	0.0	10.4	b
39. $C_3H_7 + H_2 \longrightarrow C_3H_8 + H$	9.2	0.0	15.4	b
40. $C_3H_7 + C_2H_6 \longrightarrow C_3H_8 + C_2H_5$	8.5	0.0	12.3	b
41. $C_3H_7 + C_3H_6 \longrightarrow C_3H_8 + C_3H_5$	8.0	0.0	9.8	b
42. $C_3H_7 + RH \longrightarrow C_3H_8 + R$	8.0	0.0	10.4	b
43. $C_2H_3 + H_2 \longrightarrow C_2H_4 + H$	3.24	2.0	5.11	a
44. $C_3H_5 + H_2 \longrightarrow C_3H_6 + H$	10.5	0.0	19.7	b
45. $C_3H_5 + C_2H_6 \longrightarrow C_3H_6 + C_2H_5$	8.9	0.0	20.5	b
46. $C_3H_5 + C_3H_8 \longrightarrow C_3H_6 + C_3H_7$	8.5	0.0	16.1	b
47. $C_3H_5 + RH \longrightarrow C_3H_6 + R$	8.5	0.0	16.4	b
48. $R + H_2 \longrightarrow RH + H$	9.5	0.0	15.7	b
49. $R + C_2H_6 \longrightarrow RH + C_2H_5$	8.5	0.0	12.3	b
50. $R + C_3H_8 \longrightarrow RH + C_3H_7$	8.0	0.0	10.4	b
51. $R + C_3H_6 \longrightarrow RH + C_3H_5$	8.0	0.0	9.8	b
52. $R + R'H \longrightarrow RH + R'$	8.0	0.0	10.4	b
ADDITIONS:				
53. $H + C_2H_4 \longrightarrow C_2H_5$	10.6	0.0	2.6	b
54. $H + C_3H_6 \longrightarrow C_3H_7$	9.9	0.0	2.9	b
55. $H + O_1 \longrightarrow PR_1$	9.9	0.0	2.9	b
56. $CH_3 + C_2H_4 \longrightarrow C_3H_7$	8.1	0.0	7.7	b
57. $CH_3 + C_3H_6 \longrightarrow C_4H_9$	8.5	0.0	9.1	b
58. $CH_3 + O_1 \longrightarrow PR_{1+1}$	8.3	0.0	8.9	b
ISOMERIZATIONS				
59. $2-C_5H_{11} \longrightarrow 1-C_5H_{11}$	10.7	0.0	23.4	b
60. $2-C_6H_{13} \longrightarrow 1-C_6H_{13}$	8.9	0.0	11.1	b

a. C. K. Westbrook, F. L. Dryer, and K. P. Schug, Nineteenth Symposium (Int'l) on Combustion, The Combustion Institute, 153-166 (1982) (Ref. 31).

b. D. L. Allara and R. Shaw, J. Phys. Chem. Ref. Data, 9, (3), 523-559 (1980) (Ref. 32).

acetylene, dienes, H radical, alkyl radicals and alkenyl radicals. The model
includes specific rates for species with four or less carbons and general rates
for species with 4 or more carbons. Consequently, the program can easily be
recompiled to handle arbitrarily long hydrocarbon chains but is presently
restricted to straight chain aliphatics. It would be straightforward to
incorporate the cracking of additional hydrocarbon species, such as napthene into
this model.

The cracking of normal paraffins in the temperature range of 400-1000 K is
well-described by the Rice, Kossiakoff, and Herzfeld (RKH mechanism) (33-36):
large paraffinic radicals are formed by initiation or hydrogen transfer steps and
then decompose via successive β-eliminations of 1-olefins to make methyl and ethyl
radicals. These small radicals then abstract hydrogens from the heavier paraffins
to stabilize as methane and ethane and propagate the chain reaction. In the
simplest form of this mechanism, the larger paraffinic radicals either continue to
decompose or are stabilized by abstracting hydrogens from other large paraffins.
It has been found, however, that ethylene yields (ethylene forms from radicals on
the ends of the paraffin chains) are too high from the simplest model. To correct
this shortcoming, it is assumed in the complete RKH mechanism that all radicals
with chain lengths greater than five, internally isomerize (33). Several
researchers have tested this modified mechanism and have found good agreement with
experiment (36-40).

In developing our hydrocarbon cracking model, we have tried to extend the RKH
model to higher temperatures. This has been accomplished by including mechanisms
for the decomposition of ethyl radical to ethylene (reaction 8), propyl radical to
propylene (reactions 9 and 10), vinyl radical to acetylene (reaction 12); for
hydrogen abstractions from all gas species by H radical (reactions 23 through 28)
and by larger radicals from both small and large molecules (reactions 29 through
52); and for additions to olefins by H and CH_3 radicals (reactions 53 through 58).
Rather than assuming that heavy radicals always isomerize before decomposition, we
have also included isomerization rates (reactions 59 and 60) which are used to
determine the extent of isomerization in competition with the other processes which
can create or destroy large radicals.

Many of the rate constants used in the model were taken unchanged from an
excellent compilation by Westbrook and Dryer (31) and Allara and Shaw (32). Some
of these rate constants were adjusted slightly for the following two reasons: 1)
Adjustments were made within the reported error tolerances to make the model's
predictions agree better with the experiment. 2) Since these rate constants were

collected to describe the pyrolysis of n-alkanes in the temperature range of 700-850 K, adjustments were made in the Arrhenius parameters to better fit higher temperature data while still maintaining the same rate at 775 K.

The model is solved using the steady state (SS) approximation to calculate new radical populations at the start of each integration step. According to Benson (41), steady state approximations are valid as long as radical populations are small relative to gas populations. This has been the case in all our simulations for temperatures up to 1500 K. The initial results using literature rate constants provide good agreement with data. The accuracy of the SS method has been checked by comparison to complete integration procedures using Gear's method (42).

The model involves two additional approximations which greatly simplify the computer coding and reduce the run times significantly. 1) A single termination rate constant is used and 2) only one alkyl radical and one alkenyl radical are included for each hydrocarbon chain length in the simulation. The distributions of radicals over the various carbons in each of these species are given by normalized stoichiometric coefficients. The value of the single termination rate is used as the adjustable parameter in each simulation.

The net effect of the SS and single recombination rate assumptions is that radical populations are calculated at the start of each integration step by the solution of a single quadratic equation for the total radical population and a system of linear algebraic equations for the individual radical populations. The problems associated with stiffness in the differential equations used in this kinetic model are eliminated, large time steps can be used, and computer run-times are short.

If the model of Table 7 were solved exactly for a mixture of C_{20} alkanes, coupled stiff differential equations for 59 gases (H_2, 20 alkanes, 19 alkenes, and 19 dienes) and for 283 radicals (H, 110 alkyl, and 172 alkenyl) would have to be solved. The assumptions of steady state conditions and a single termination rate constant reduce the problem to 59 coupled nonstiff differential equations for the gases, a quadratic equation for R_{total}, and solution of a system of 282 linear algebraic equations for the radicals. Introduction of the stoichiometric coefficients further reduces the algebraic equations to a system of 40 linear equations for the radicals (H, 20 alkyl, 19 alkenyl) and iterative solution of 277 equations for the coefficients. The net effect of all three approximations is an enormous decrease in computer run-times.

For a model describing the cracking of mixtures of n-alkanes up through C_8, accurate simulations for temperatures up to 1500 K can be run on a PDP 11/23 laboratory minicomputer in less than 15 minutes. Run times have been decreased by nearly a factor of 10 on a Sun or Apollo workstation. These short run-times have greatly aided in debugging and validating the current model.

The model needs, as inputs, the temperature-time profile for the reactor (obtained from the heat transfer model discussed below), initial concentrations, the pressure, and the integration step size. A standard kinetics file is used for all simulations. Outputs from the model are: calculated time, temperature, gas concentrations (H_2, paraffins, olefins, acetylene and dienes), radical concentrations (H, alkyl, alkenyl and total) and radical reaction velocities for all the categories of reactions listed in Table 7.

Simulations have been carried out for both in-house and literature data and the results are generally in good agreement with experiment (43,44). In Fig. 62, comparisons between theory and experiment are presented for the pyrolysis of ethane at several temperatures. These data were collected in the entrained flow reactor at AFR using in-situ FT-IR analysis. Good results were also obtained fitting data on shock tube pyrolysis of octane (Doolan and Mackie, 45), as shown in Fig. 63. In Fig. 64 results of simulations for the cracking of hexadecane at 68 atm (1000 psig) pressure are presented. These are compared with the data of Fabuss and coworkers (46), for carbon number distribution. Data and simulations are presented in Fig. 65 for atmospheric pressure pyrolysis of Solpar (47), a mixture of C_{12}-C_{18} n-alkanes. In this case the products are predominantly olefinic at high conversions.

Additional details of the hydrocarbon cracking model are given in the paper "A Kinetic Model for the Pyrolysis of Large N-Alkanes," which is included as Appendix C.

For the purpose of combining this model with the soot submodel in the next section, first the reactions involving C_2H_2, C_2H_4, C_2H_3, were removed and replaced with the corresponding reactions from the soot submodel. The consequence of this will be discussed below.

Soot Model

Our initial approach to extending the hydrocarbon cracking model to soot formation was to add reactions for the growth of polyacetylenes (25) to the existing hydrocarbon cracking model. This did not work because the approximations
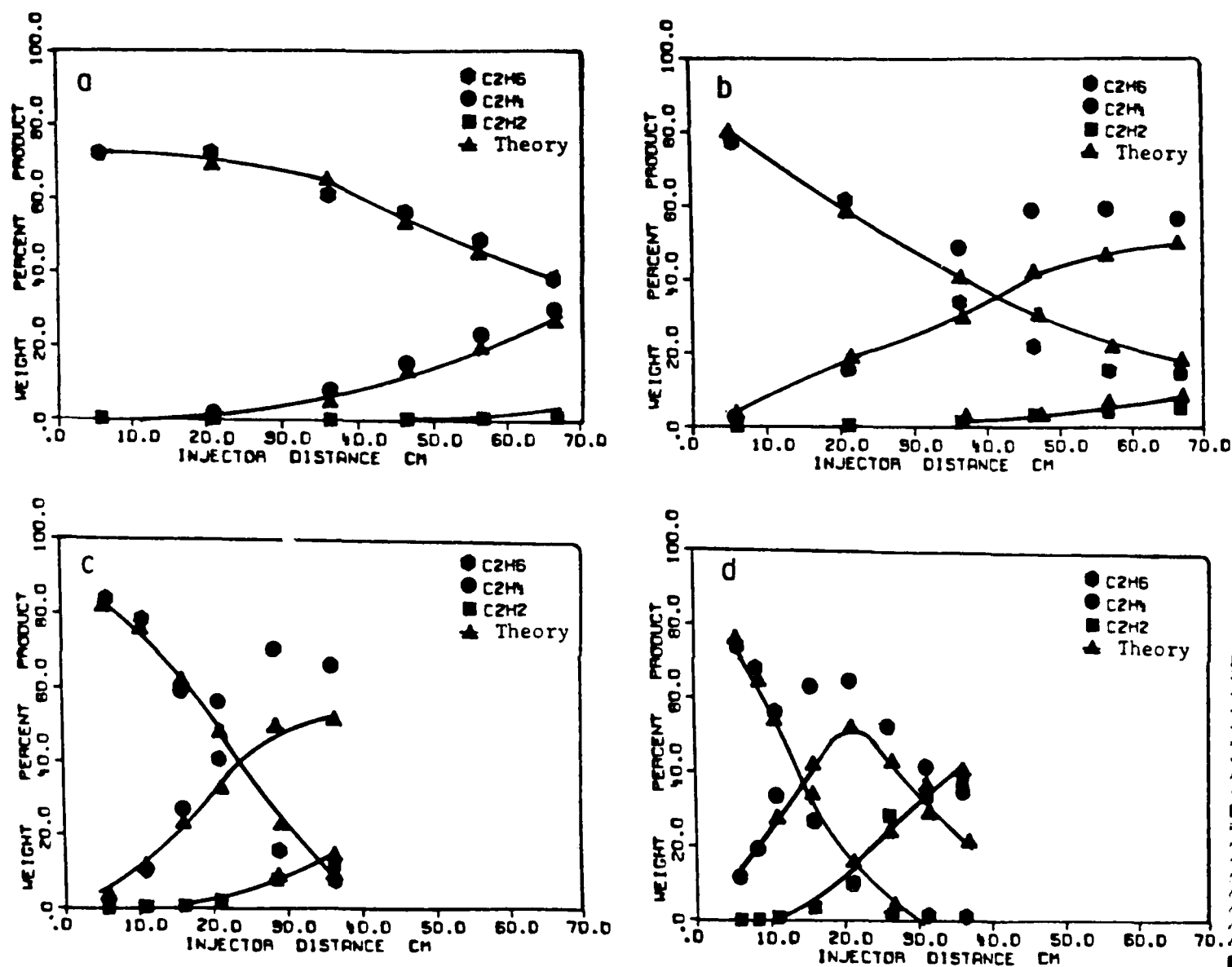
Figure 62. Pyrolysis of Ethane at Several Temperatures, Experiment (symbols) and Theory (lines). Gas Velocity = 1 m/sec, Pressure = 1 atm, Concentration = 1.2 x 10^{-4} moles/liter. a) 800°C, b) 900°C, c) 1000°C, and d) 1100°C.
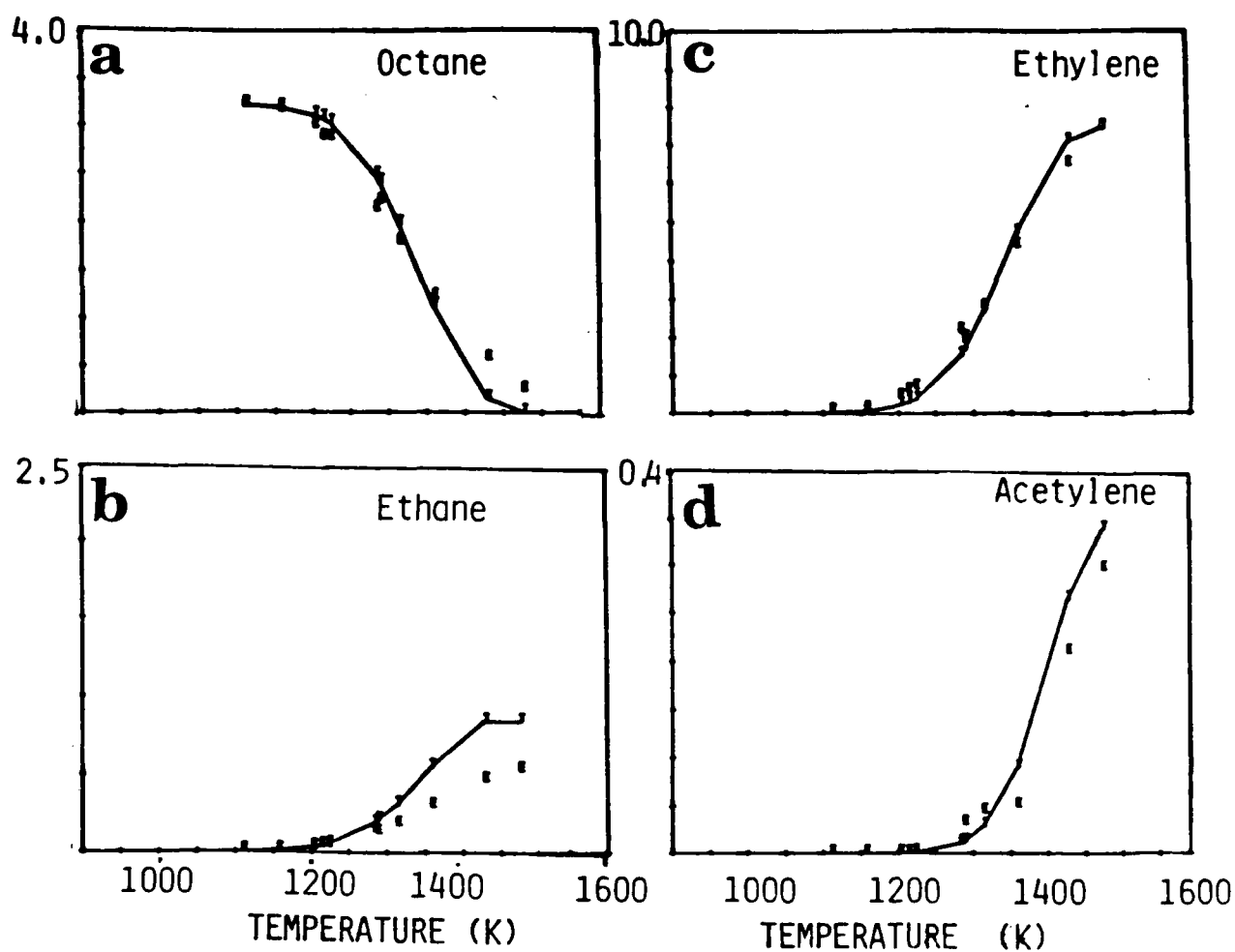
Figure 63. Shock-Tube Pyrolysis of Octane Using Modified Initiation Rates (45). Experiment (E) and Theory (T).
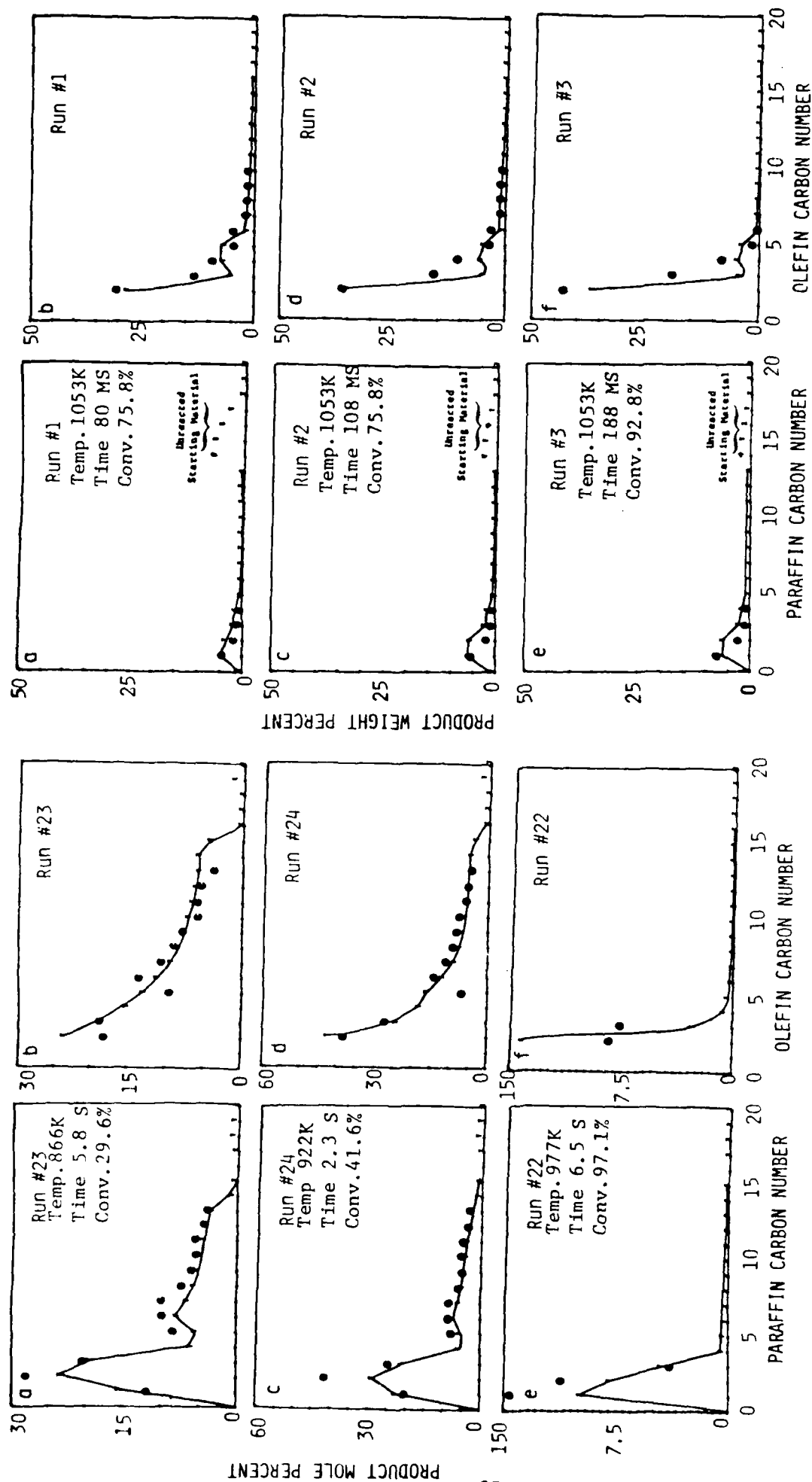
Figure 64. Paraffin and Olefin Carbon Number Distribution from Thermal Cracking of Hexadecane at 68 atm. Symbols: (●) - Experimental Data; (T) - Predictions of Cracking Model. Solid Lines Connect Model Predictions. Data from Ref. 38.

Figure 65. Paraffin and Olefin Carbon Number Distribution from the Thermal Cracking of Solpar (a commercial mixture of C_{12} - C_{18} n-alkanes). Symbols: (●) - Experimental Data; (T) - Predictions of Cracking Model. Solid Lines Connect Model Predictions. All Runs were done in Steam at Slightly above 1 atm Pressure. Data from Ref. 39.

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used in the solution of this model break down with the addition of these additional
species and reactions (steady-state radical populations, independent isomerization
of radicals). The major "bad-actor" species for the steady-state approximations
were C_2H_2 and C_2H. At low temperature the radical C_2H was in steady-state
equilibrium with the C_2H_2, but at high temperature the reverse occurred, with the
C_2H_2 appearing to be in chemical equilibrium with the radicals.

With this background then, we obtained a Gear's method integration package
from Dr. Ripudaman Malhotra of Stanford Research Institute. This package was
written by Gary Z. Whitten of Systems Applications, Inc. and incorporates the Gear
integration package of Hindmarsh (48). The version we obtained was modified to run
on a DEC PDP11. At the time of our initial work on this, we were limited to the
use of a small PDP 11/23 microcomputer, which allowed the use of only 40 species
and 100 explicit reactions. With the acquisition of larger workstations (Sun
3/260), we have now modified this package to run under UNIX and to use 400
reactions, and 100 species, and now the code includes the computation of reverse
reactions from thermodynamic tables in the NASA format.

Because of these initial computer limitations our initial reaction set of 33
soot reactions were those of Tanzawa and Gardiner (24) for acetylene and Kiefer
(25) for ethylene, together with a very small number of reactions from Frenklach,
et al.'s (23,49-53) soot model for the production of soot. From this base, we
approached the current form of the model, which is basically a subset of Frenklach
et al.'s model with additional reactions for the cracking of long chain
hydrocarbons, based on the hydrocarbon cracking submodel. Frenklach's model is
based on Tanzawa and Gardiner's acetylene model, which leads to polyacetylenes.
The rest of Frenklach's mechanisms included most of the likely radical atom
reactions. His work uses literature values for initiation reactions (where
available) and rate classes for the rest. The rate for each class was determined
from either a literature value for a prototype reaction in the class, or from an
upper limit based on collision theory if no experimental data was available. That
work identified several possible pathways to soot, mainly involving the addition of
acetylene or hydrogen to intermediate species. Based on this result, we selected
only those species and reactions, that were on these few pathways of interest, and
all species not directly involved in the main pathways. This eliminated isomers
which do not react in the pathway, which should increase reaction velocities for
the pathways.

The reaction scheme we use is shown in Table 8. It includes most of the
species we see experimentally with the exception of any C_3's. It includes:

Table 8 - Soot Model.

(units are in μliters, moles, μsecs, °K)

No.	Reaction	Rate Class	A	E(°K)	n
1	C2H6 = CH3 + CH3	0	5.0119E+10	4.4791E+04	0.00
2	C3H8 = CH3 + C2H5	0	7.9430E+10	4.2828E+04	0.00
3	C4H10 = CH3 + C3H7	0	3.1600E+11	4.3130E+04	0.00
4	C5H12 = CH3 + C4H9	0	6.3090E+10	4.2979E+04	0.00
5	C4H10 = C2H5 + C2H5	0	2.5188E+10	4.1318E+04	0.00
8	C2H5 = C2H4 + H	0	3.9811E+07	2.0382E+04	0.00
9	C3H7 = CH3 + C2H4	0	1.2589E+07	1.6356E+04	0.00
10	C4H9 = C2H5 + C2H4	0	2.5119E+07	1.4494E+04	0.00
11	C2H4 + H = C2H5	0	3.9811E+10	1.3080E+03	0.00
12	C2H4 + CH3 = C3H7	0	1.2589E+08	3.8750E+03	0.00
13	H2 + C4H9 = H + C4H10	0	3.1623E+09	7.9014E+03	0.00
14	H2 + R4-2 = H + C4H10	0	3.1623E-09	7.9014E+03	0.00
15	CH4 + C4H9 = CH3 + C4H10	0	1.2580E+09	9.2099E+03	0.00
16	CH4 + R4-2 = CH3 + C4H10	0	1.2580E+09	9.2099E+03	0.00
17	C2H6 + C4H9 = C2H5 + C4H10	0	5.0100E+08	6.1902E+03	0.00
18	C2H6 + R4-2 = C2H5 + C4H10	0	5.0100E+08	6.1902E+03	0.00
19	CH4 + H = H2 + CH3	0	2.5119E+10	5.7373E+03	0.00
20	C2H6 + H = H2 + C2H5	0	1.2589E+11	4.8817E+03	0.00
21	H + C4H10 = H2 + C4H9	0	1.2589E+11	3.8752E+03	0.00
22	H + C4H10 = H2 + R4-2	0	1.2589E+11	3.8752E+03	0.00
24	CH3 + H2 = CH4 + H	0	1.5849E+09	5.6870E+03	0.00
25	CH3 + C2H6 = CH4 + C2H5	0	6.3096E+08	5.8379E+03	0.00
26	CH3 + C4H10 = CH4 + C4H9	0	3.9811E+08	4.8314E+03	0.00
27	CH3 + C4H10 = CH4 + R4-2	0	3.9811E+08	4.8314E+03	0.00
29	H2 + C2H5 = C2H6 + H	0	3.9811E+09	7.0450E+03	0.00
30	CH4 + C2H5 = C2H6 + CH3	0	7.9433E+08	8.9582E+03	0.00
31	C2H5 + C4H10 = C2H6 + C4H9	0	1.5849E+08	5.2340E+03	0.00
32	C2H5 + C4H10 = C2H6 + R4-2	0	1.5849E+08	5.2340E+03	0.00
35	H + H = H2 (M)	40	1.0000E+10	0.0000E+00	0.00
36	CH3 + H = CH4	0	2.0000E+10	0.0000E+00	0.00
37	C2H5 + H = C2H6	0	2.0000E+10	0.0000E+00	0.00
38	H + C3H7 = C3H8	0	2.0000E+10	0.0000E+00	0.00
39	H + C4H9 = C4H10	0	1.0000E+10	0.0000E+00	0.00
46	CH3 + CH3 = C2H6	0	2.0000E+10	0.0000E+00	0.00
47	CH3 + C2H5 = C3H8	0	2.0000E+10	0.0000E+00	0.00
48	CH3 + C3H7 = C4H10	0	2.0000E+10	0.0000E+00	0.00
49	CH3 + C4H9 = C5H12	0	1.0000E+10	0.0000E+00	0.00
56	C2H5 + C2H5 = C4H10	0	2.0000E+10	0.0000E+00	0.00
57	C2H5 + C3H7 = C5H12	0	2.0000E+10	0.0000E+00	0.00
58	C3H7 + C3H7 = C4H10	0	1.0000E+10	0.0000E+00	0.00
65	C3H7 + C3H7 = C4H9	0	2.0000E+10	0.0000E+00	0.00
66	C3H7 + C4H9 = R7-4	0	2.0000E+10	0.0000E+00	0.00
73	C4H9 + R7-4 = H	0	1.0000E+10	0.0000E+00	0.00
100	R7-4 + M = C2H2 + C2H2	0	1.2600E+36	2.5458E+04	-7.17
101	C2H3 + C2H2 = C4H4 + H	0	1.5849E+10	1.2624E+04	0.00
102	C2H3 + C4H4 = A1- + H	13	0.0000E+00	0.0000E+00	0.00
103	C2H3 + C4H5U = A1 + H	-5	0.0000E+00	0.0000E+00	0.00
104	C4H5U + C4H4 = A1C2H2U + H2	2	0.0000E+00	0.0000E+00	0.00
105	C4H4 + H = C4H3U + H2	0	3.9811E+10	0.0000E+00	0.00
106	C4H4 + C2H = C4H3U + C2H2	0	0.0000E+00	0.0000E+00	0.00
107	C4H3U + C2H2 = C6H5U	13	0.0000E+00	0.0000E+00	0.00
108	C6H5U + C2H2 = A1-	30	0.0000E+00	0.0000E+00	0.00
109	A1- + H2 = A1 + H	-23	0.0000E+00	0.0000E+00	0.00
110	A1- + C2H2 = A1C2H2U	0	0.0000E+00	0.0000E+00	0.00
111	A1C2H2U + H = A1C2H + H2	0	0.0000E+00	0.0000E+00	0.00
112	C2H + H2 = C2H2 + H	0	1.1200E+10	1.4430E+03	0.00
113	C2H + C2H2 = C4H2 + H	0	3.9811E+10	0.0000E+00	0.00
114	C2H + C4H2 = C6H2 + H	0	3.9811E+10	0.0000E+00	0.00

Table 8 - Soot Model. (continued)

(units are in μliters, moles, μsecs, °K)

No.	Reaction	Rate Class	A	E(°K)	n
116	C4H3U + M = C4H2 + H	0	1.0000E+13	3.0058E+04	0.00
117	C4H4 + M = C4H3U + H (REV)	0	1.0000E+15	0.0000E+00	0.00
118	C4H4 = C2H2 + C2H2	0	1.2990E+12	4.1505E+04	0.00
119	C2H2 + M = C2H + H	0	4.1687E+13	5.3865E+04	0.00
120	H2 + M = H + H	0	2.2387E+09	4.6531E+04	0.50
121	C4H2 + M = C4H + H	0	3.4674E+14	4.0279E+04	0.00
122	C4H + C2H2 = C6H2 + H	0	3.9811E+10	0.0000E+00	0.00
124	C6H2 + M = C6H + H	0	5.0119E+13	4.0279E+04	0.00
127	C2H4 + M = C2H2 + H2	0	2.5100E+14	3.9889E+04	0.00
128	C2H4 + M = C2H3 + H	0	4.0000E+14	4.9389E+04	0.00
129	C2H4 + H = C2H3 + H2	2			
130	H + C2H3 = H2 + C2H2	32			
131	C4H2 + H = C4H + H2	-1			
132	C6H2 + H = C6H + H2	-1			
134	C2H2 + C2H = C4H3U	8			
135	C4H2 + C4H3U = C4H + C4H4	-4			
136	C2H + C4H2 = C2H2 + C4H	3			
137	C2H + C6H2 = C2H2 + C6H	3			
138	C4H + C4H2 = C6H2 + C2H	-10			
141	C2H2 + C2H3 = C2H4 + C2H	-4			
142	C2H3 + C4H2 = C2H + C4H4	12			
143	C2H3 + C4H2 = C2H4 + C4H	-4			
144	H + C4H3U = H2 + C4H2	32			
145	C4H5U + H = C4H4 + H2	32			
146	C6H5U + H = C6H6	29			
147	C6H6 + H = C6H5U + H2	2			
148	C6H6 + C2H = C6H5U + C2H2	4			
149	C4H3U + C2H3 = C6H6	7			
150	C4H5U + C2H2 = C6H7U	13			
151	C6H6 + H = C6H7U	5			
152	C6H7U + H = C6H6 + H2	32			
153	A1- + H = A1	-21			
154	A1- + C2H = A1C2H	7			
155	A1 + C2H = A1- + C2H2	24			
156	A1 + C4H = A1- + C4H2	24			
157	A1C2H + H = A1- + C2H2	25			
158	A1C2H + C2H = A1- + C4H2	-26			
159	C6H7U + H = A1 + H2	20			
160	A1C2H* + H = A1C2H + H2	-21			
161	A1C2H + H = A1C2H* + H2	23			
162	A1C2H + C2H = A1C2H* + C2H2	24			
163	A1C2H* + C2H2 = A1C2HAC	127			
171	H + A1C2H- = A1C2H	-21			
172	H2 + A1C2H- = A1C2H + H	-23			

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Table 8 - Soot Model. (concluded)

(units are in μliters, moles, μsecs, °K)

	Reaction					Rate Class	A	E(°K)	n
173	C2H2	A1C2H-	=	A1C2H	C2H	-24			
174	H	A1C2H2U	=	A1C2H3	H	29			
175	H2	A1C2H2U	=	A1C2H3		-2			
176	C2H2	A1C2H2U	=	A1C4H4U	A1C4H3	13			
177	A1C4H4U		=	H	A2	20			
178	A1C4H4U		=	H	A1C4H3	-5			
179	A1C4H4U	H	=	A1C4H5	H	29			
180	A1C4H4U	H2	=	A1C4H5	H2	-2			
181	A1C4H4U	C2H2	=	A1C4H5	C2H2	-4			
182	A2-	H	=	A2	H	-21			
183	A2-	H2	=	A2	H2	-23			
184	A2-	C2H2	=	A2	C2H	-24			
185	A1C2HAC		=	A2-X		30			
186	H	A2-X	=	A2	H	-21			
187	H2	A2-X	=	A2	H2	-23			
188	C2H2	A2-X	=	A2	C2H	-24			
189	H	A1	=	R6%		19			
190	R6%		=	C6H7U		-20			
191	A2-X	C2H2	=	H	A2R5	127			
192	H	A2R5-	=	A2R5	H	121			
193	C2H2	A2R5-	=	A2R5	C2H	-124			
194	H2	A2R5-	=	A2R5	H	-123			
195	C2H	C6H7U	=	C2H2	C6H6	32			
196	C2H	C4H5U	=	C6H6		7			
197	C2H	C2H	=	C4H2		7			
198	C2H	C4H	=	C6H2		7			
201	C2H	C4H4	=	C4H4		7			
202	C2H3	C6H2	=	C4H	C2H4	12			
203	C2H3	C6H2	=	C6H	C6H6	-4			
204	C2H3	C4H4	=	H	C4H4	16			
205	C2H	C2H4	=	H	A1	17			
206	C6H2	A1-	=	C6H	A1C2H	-24			
207	C6H2	A1-	=	C4H	A1C2H2U	26			
208	A1C4H5		=	C2H3	A1C2H2U	-7			
209	C4H2	A1C2H2U	=	C4H	A1C2H3	-4			
210	A1C4H3		=	A1-	C4H3U	-7			
211	C2H	A1C4H3	=	A1C4H3	C2H2	7			
212	C2H3	C2H2	=	C2H2	C2H2	0			
213	C4H4	C4H3U	=	C2H4	C2H4	15			
249	AR		=			0	1.0000E+10	0.0000E+00	0.00

Tanzawa and Gardiner's polyacetylene reactions (24) with the exception of the
C_8's; Kiefer's ethylene reactions (25) again with the exception of the C_8's;
Kiefer's recent initiation reaction (54) (reaction 118 in Table 8); two basic
pathways to the first aromatic ring; and most of the reactions leading to
acenaphthalene. The notation for the species is that of Frenklach (23,49-53).

Frenklach (53) identified two routes to the formation of the first aromatic
ring, a dominant one via the C_6H_5 radical (reaction 108 and associated reactions)
and the other via the C_6H_7 radical (reaction 159, etc). Other workers, Colket
(55), Harris (56), among others, have also used these pathways. For the shock tube
studies of those workers the C_6H_5 path was found to be the dominant one. We have
found, however, for our slow long residence time pyrolyses, that the C_6H_7 pathway
is needed to obtain significant quantities of benzene in the simulation.

Similarly, Frenklach (53) identified two pathways from the first to the second
ring, and found one to be dominant.

Again, we found it necessary to add the "minor" route in order to obtain
significant quantities of "soot." This is the mechanism proposed by Bittner and
Howard (57).

The soot growth modeling is ended at acenaphthalene, because it is the first
major "island of stability". For purposes of comparison with our FT-IR
experiments, we plot everything heavier than benzene (A_1) as "soot", since that is
essentially the grouping of our experimental data (including tar).

The rates used for the model are listed in Table 8 for the initiation steps,
and in Table 9 for the class rates. The initiation rates are taken from
Frenklach, et al. (23) and are mainly from the literature of experimental
measurements (24,54,58-61). The class rates are also from Frenklach (53) with the
exception of class 23, H abstraction of aryl H, and class 27, aryl additions to
triple bonds, which were reduced to agree with more recent information.

The model in Table 8 can be broken into three parts: the first part is taken
from the hydrocarbon cracking model for butane (reactions 1 through 100). For this
part of the model, reverse reactions are entered explicitly, as are the rates for
the forward and reverse reactions (mainly Refs. 32 and 33 as discussed under the
cracking model). The second and third parts follow Frenklach and use the principle
of detailed balance and thermodynamics to calculate the reverse rates, with the
rates limited to 1×10^{11} μl/mole/μsec for bimolecular reactions involving H atom

Table 9 - Reaction Rate Classes. (see Frenklach Ref. for definitions and references) Units are μliters, moles, μsecs, °K.

Reaction Class	A	E(°K)
1	0.35000e+10	0.10580e+04
2	0.15000e+12	0.51340e+04
3	0.20000e+11	0.00000e+00
4	0.20000e+11	0.00000e+00
5	0.55000e+10	0.12024E+04
6	0.10000e+11	0.75780e+03
7	0.10000E+11	0.00000e+00
8	0.10000E+11	0.00000e+00
9	0.20000E+11	0.00000e+00
10	0.10000E+11	0.00000e+00
11	0.16000E+11	0.12630e+05
12	0.10000E+11	0.00000e+00
13	0.10000E+11	0.00000e+00
14	0.10000E+11	0.00000e+00
15	0.10000E+10	0.81794e+04
16	0.10000E+08	0.40897e+04
17	0.60000E+09	0.19246e+04
18	0.10000E+00	0.00000e+00
19	0.10000E+11	0.75780e+03
20	0.10000E+05	0.00000e+00
21	0.20000E+12	0.59730e+05
22	0.10000E+11	
23	0.25000E+12	0.80520e+04
24	0.20000E+11	0.00000e+00
25	0.10000E+12	0.00000e+00
26	0.20000E+11	0.00000e+00
27	0.20000E+10	0.00000e+00
28	0.20000E+11	0.00000e+00
29	0.20000E+11	0.00000e+00
30	0.10000E+05	0.00000e+00
31	0.10000E+11	0.00000e+00
32	0.10000E+11	0.00000e+00
33	0.20000E+11	0.00000e+00
34	0.00000E+11	0.00000e+00
35	0.00000E+11	0.00000e+00
36	0.00000E+11	0.00000e+00
37	0.00000E+11	0.00000e+00
40	0.0	0.0

and $2 \times 10^{10} \mu$l/mole/μsec for reactions that do not involve H. The second part of the model are the reactions for which explicit rates have been measured and the third part are those for which class rates are used. In Table 8, the reaction class is shown for each reaction, with 0 indicating that the rate is given in the subsequent columns, and non-zero indicating a reference to Table 9. A minus rate class means that the reverse rate is given, while a rate class >100 or <-100 indicates a one-way reaction. The one-way reactions are an artifact to allow for the lack of reactions beyond acenaphthalene.

Since one of the key initiation steps is that obtained from the experiments of Kiefer and presented at the 21st Symposium (54), for consistency we have used the same thermodynamics as he used in determining the rate. Professor Frenklach was kind enough to send us a copy of his thermodynamics (the S8 set) (50) for use in this modeling. This thermodynamic database is computed from the group additivity rules (62,63). This particular set has bond disassociation energies of 102 and 120, kcal/mole for the H-C_2H, and H-C_2H_3 bonds, respectively, and a group value of 25.57 kcal/mole for the C_t -(C_t) group (50).

Modeling Results

The model of Table 8 has been used to simulate the pyrolysis of butane at 1100°C and 1300°C, butane + H_2, acetylene and benzene at 1300°C. These results, together with the experiment pyrolysis results are shown in Figs. 66 through 70. The agreement is reasonable except for the onset of sooting, given the fact that the competing side reactions were eliminated, and the fact that this reaction scheme and rates were developed for modeling shock tube data. The agreement for the light species is of the correct order of magnitude and is usually within a factor of two to five for the major species.

In order to obtain a good degree of fit, the class rate (21) for initiation of phenyl and H atoms from benzene was increased by a factor of 100 in the simulations shown. This has a significant effect on the soot production (all the reactions leading to the second ring) and causes the agreement with experiment for soot to be quite good. The lack of the biphenyl reactions should have no effect on the acetylene pyrolysis, so the under prediction of soot with the measured phenyl recombination rate is probably due to lack of knowledge of rates, or to the uncertainty in the thermodynamics. The sensitivity of these computations to the choices made for the thermodynamics data is well known, but we have found indications that this may not be as strong a sensitivity for our pyrolyses as for the shock tube experiments. We have not done a proper sensitivity analysis, but

Butane Pyrolysis Data (1100°)
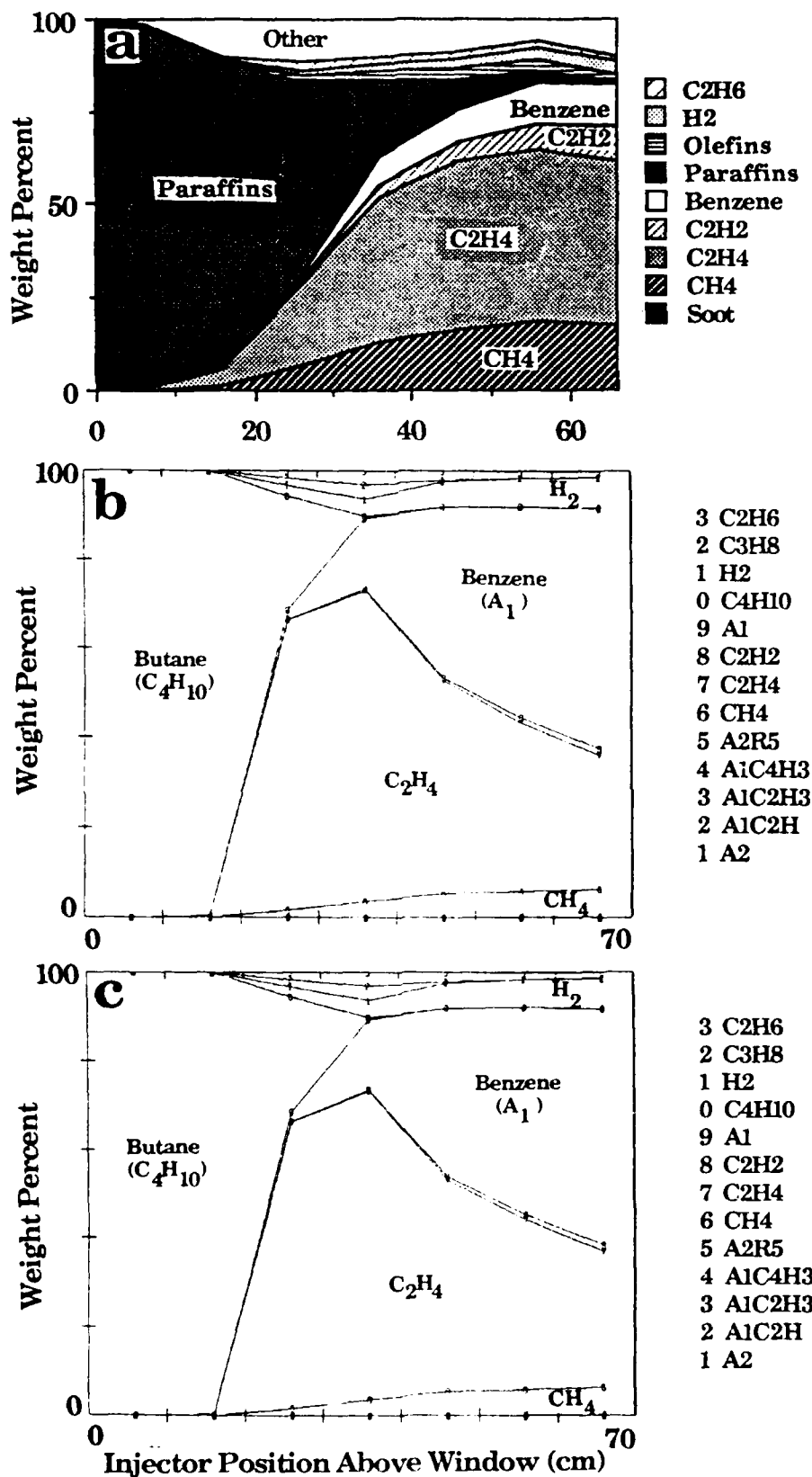
Figure 66. Comparison of Experiment with Simulations for Butane Pyrolysis at 1100°C as a Function of Reaction Distance.
a) Experimental Data, b) Simulation with Rates of Table 9 and
c) Simulation with Class Rate 21 Increased by Factor of 100.

Butane Pyrolysis Data (1300°)

a

Weight Percent

Other

Benzene

Paraffins

C2H2

C2H4

CH4

Soot

▨	C2H6
▨	H2
▤	Olefins
■	Paraffins
□	Benzene
▨	C2H2
▨	C2H4
▨	CH4
■	Soot

b

Weight Percent

H₂

Butane (C₄H₁₀)

Benzene (A₁)

C₂H₄

CH₄   Soot

3 C2H6
2 C3H8
1 H2
0 C4H10
9 Al
8 C2H2
7 C2H4
6 CH4
5 A2R5
4 A1C4H3
3 A1C2H3
2 A1C2H
1 A2

c

Weight Percent

Other   H₂

Butane (C₄H₁₀)

Benzene (A₁)

C₂H₄

CH₄   Soot

3 C2H6
2 C3H8
1 H2
0 C4H10
9 Al
8 C2H2
7 C2H4
6 CH4
5 A2R5
4 A1C4H3
3 A1C2H3
2 A1C2H
1 A2

Injector Position Above Window (cm)
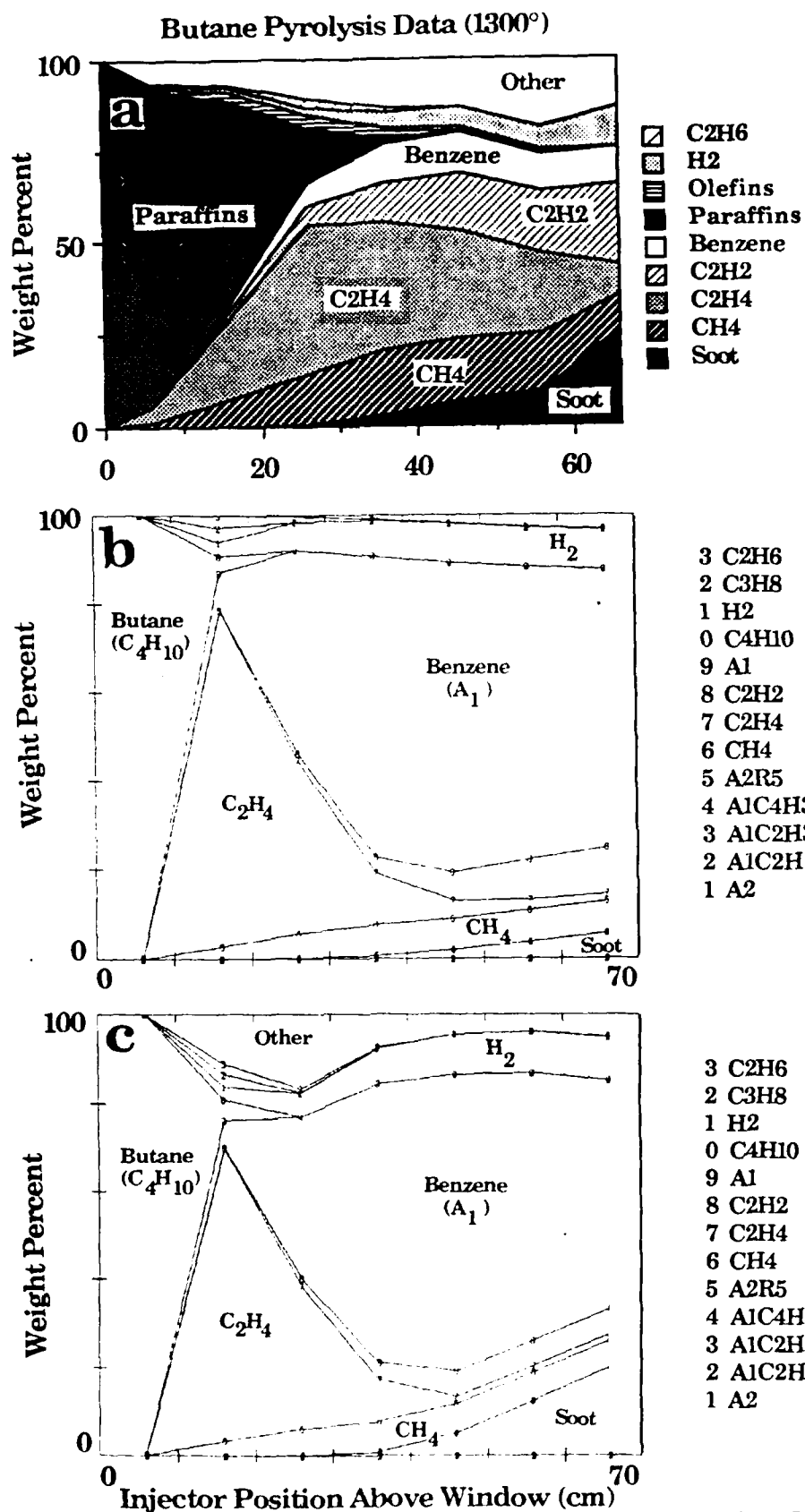
Figure 67. Comparison of Experiment with Simulations for Butane Pyrolysis at 1300°C as a Function of Reaction Distance. a) Experimental Data. b) Simulation with Rates of Table 9 and c) Simulation with Class Rate 21 Increased by Factor of 100.

Butane Plus H2 1300°C
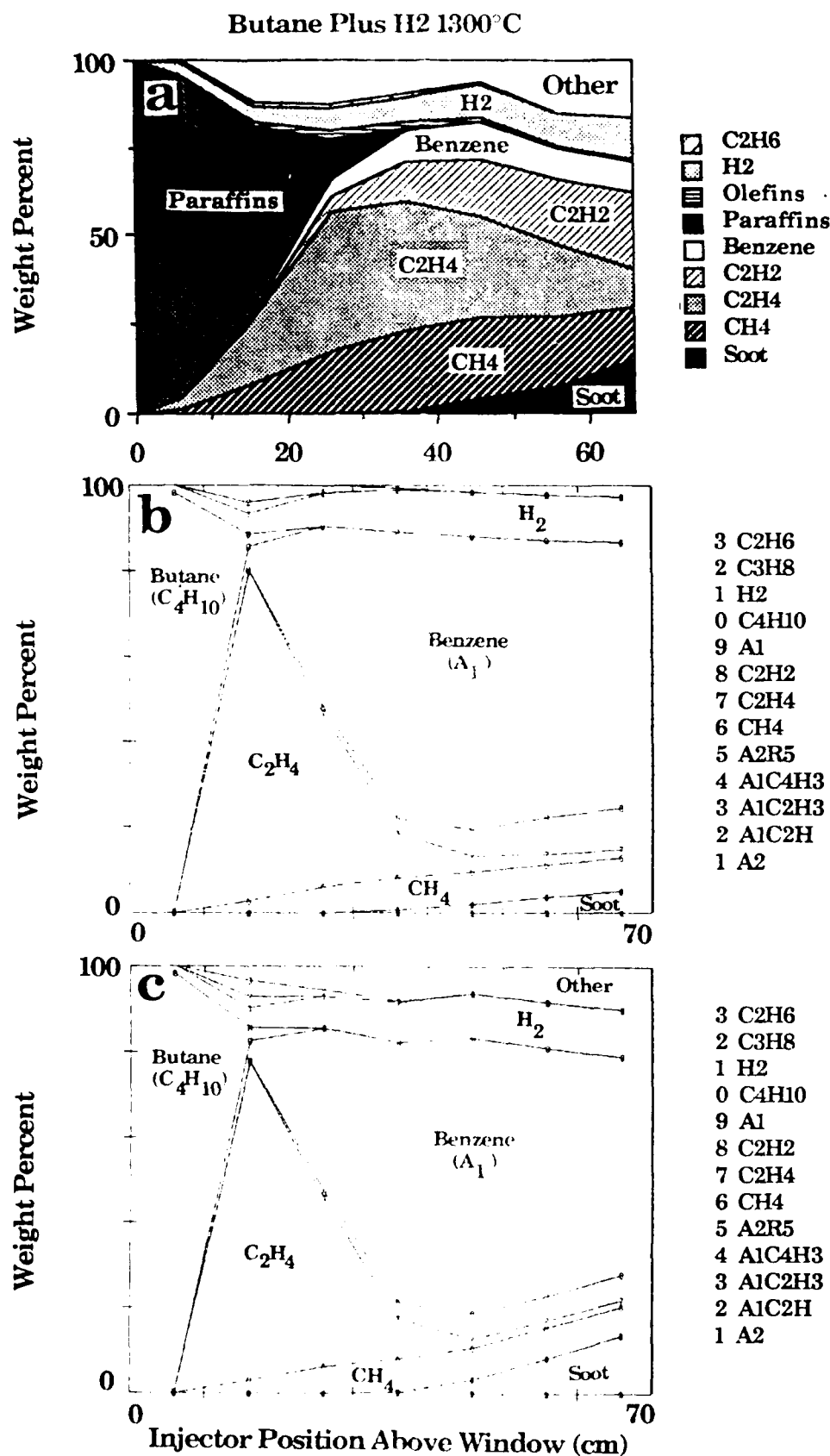
Figure 68. Comparison of Experiment with Simulations for Butane Plus Hydrogen Pyrolysis at 1300°C as a Function of Reaction Distance. a) Experimental Data, b) Simulation with Rates of Table 9 and c) Simulation with Class Rate 21 Increased by Factor of 100.
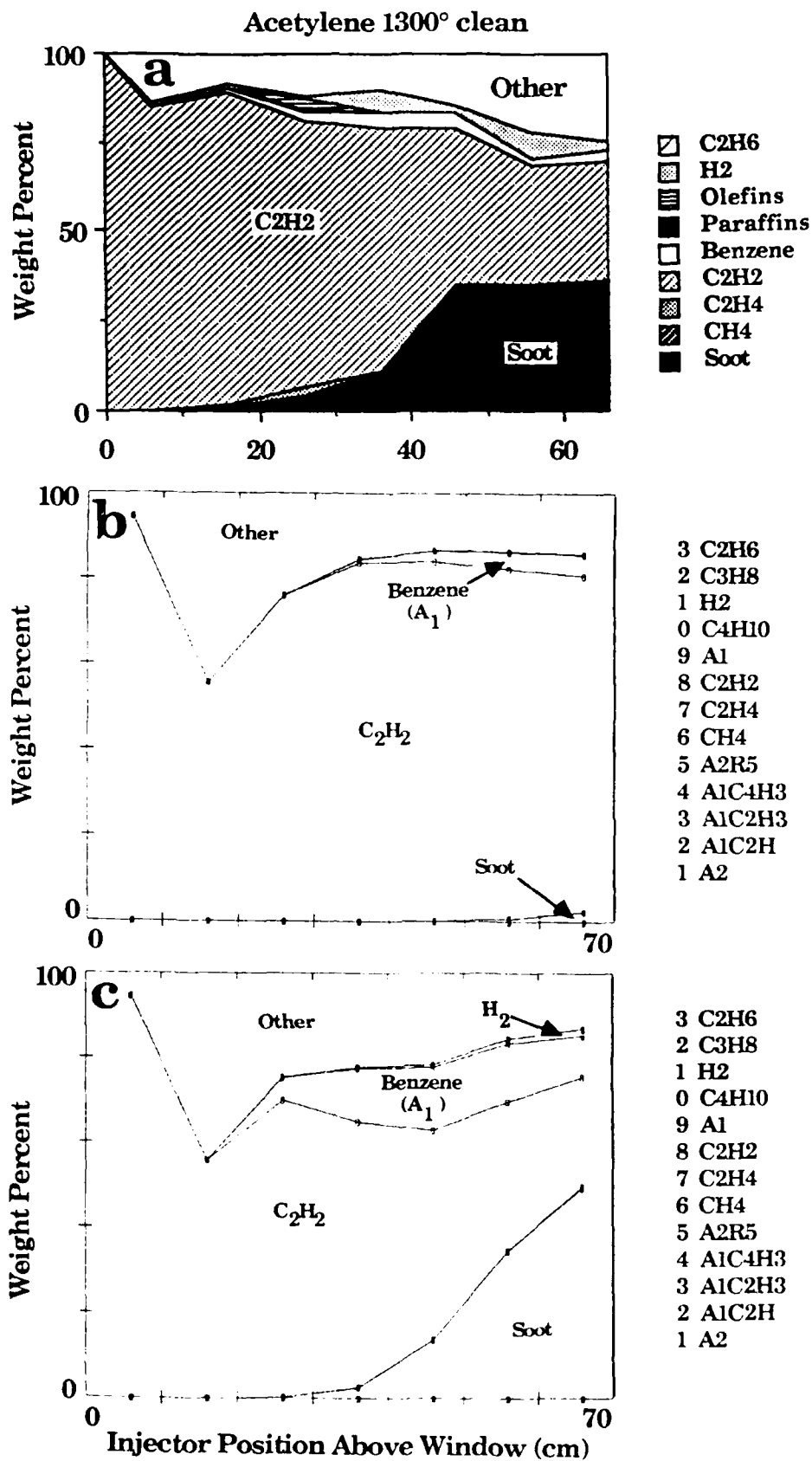
Figure 69. Comparison of Experiment with Simulations for Acetylene Pyrolysis at 1300°C as a Function of Reaction Distance. a) Experimental Data, b) Simulation with Rates of Table 9 and c) Simulation with Class Rate 21 Increased by Factor of 100.
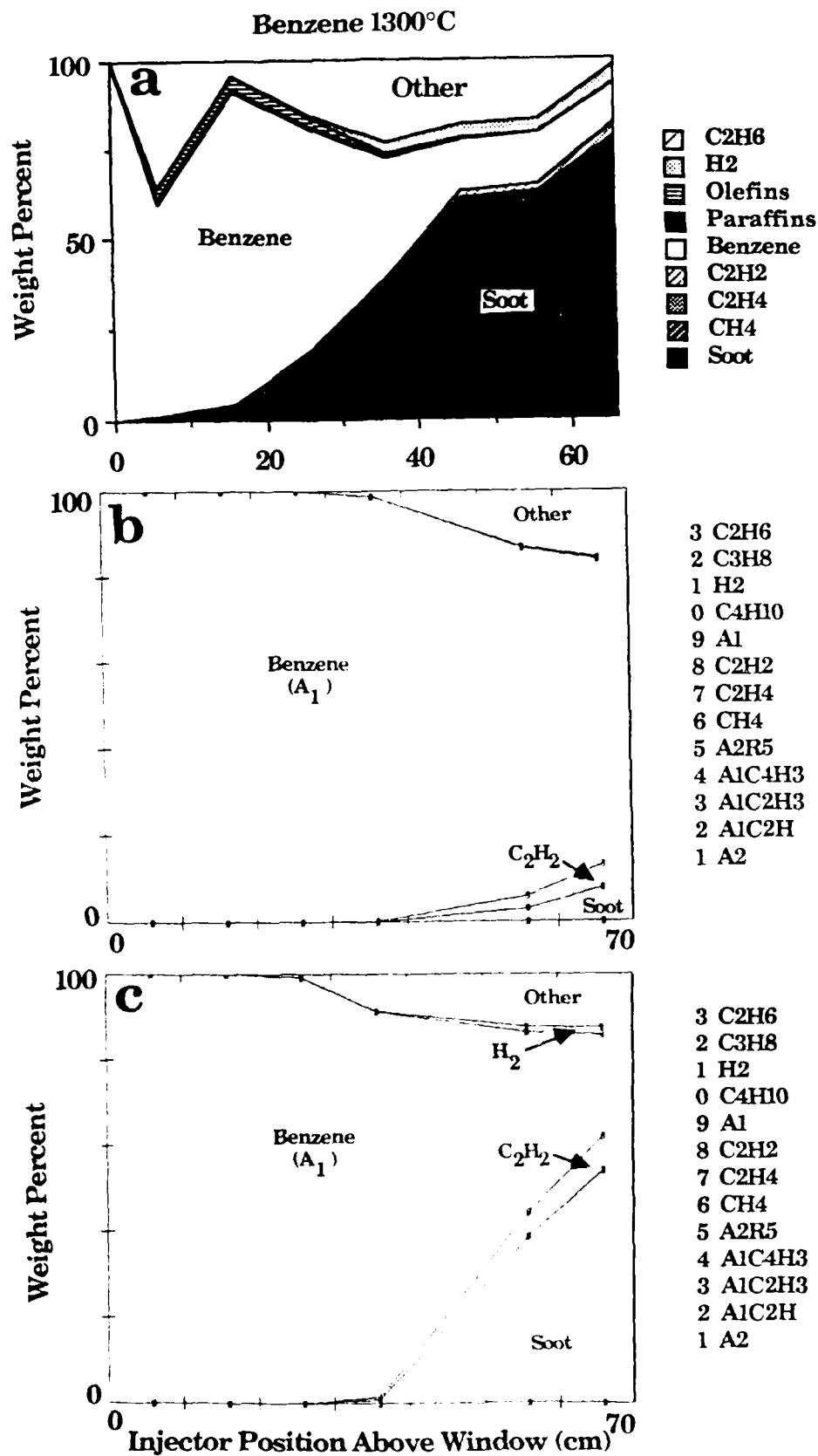
Benzene 1300°C

Figure 70. Comparison of Experiment with Simulations for Benzene Pyrolysis at 1300°C as a Function of Reaction Distance.
a) Experimental Data, b) Simulation with Rates of Table 9 and
c) Simulation with Class Rate 21 Increased by Factor of 100.

during the development of this model we have used a variety of thermodynamic data sets and gotten similar results.

For butane, the onset of soot occurs in the right place and the relative amounts CH_4, C_2H_4 and benzene are reasonable. The initial cracking of butane to form ethylene is too fast, but this effect was present in the original hydrocarbon cracking model, and can be attributed to the neglect of the endothermic reaction heat. Doubling the specific heat of butane to simulate the heat of reaction cuts the effective cracking rate in half and gives good agreement for the 16 cm simulation in Figs. 66 and 67. A similar effect is apparent in the acetylene simulation (Fig. 69).

The benzene pyrolysis simulation (Fig. 70) does not include the biphenyl formation reaction, and thus may be seriously under-predicted. It has been suggested that this reaction is not needed because enough benzene decomposes to form the acetylene and vinyl needed to build up the second aromatic ring. In any case, the benzene simulation is not bad.

Heat Transfer Model

A heat transfer model was developed for the atmospheric pressure entrained flow reactor (EFR). The model was used to simulate the time-temperature history experienced by an average hydrocarbon molecule injected into the EFR at a specified set of conditions. The development was based on a successful model used to model coal particle time-temperature histories in the same reactor. The major difference is that the coal particles are largely confined to the center of the 2 inch diameter reactor by virtue of their greater mass, while hydrocarbon molecules rather quickly diffuse to the reactor walls.

The version of the model used in the current program included an adjustable parameter, , which controlled the rate of mixing of the hydrocarbon with the N_2 main gas. The value of was chosen for each injector position in order to best match the average gas temperature at the reactor window, as measured by FT-IR emission spectroscopy.

Figure 71 presents an example of a normalized emission (emission/(1-transmission)) overlayed with a theoretical black-body temperature of 1040 K. Fairly good black-body shape is achieved in the spectral regions where the hot hydrocarbon gases absorb and, hence, emit radiation. Figure 70 compares the temperature indicated by the hot stream for each reaction distance with that of
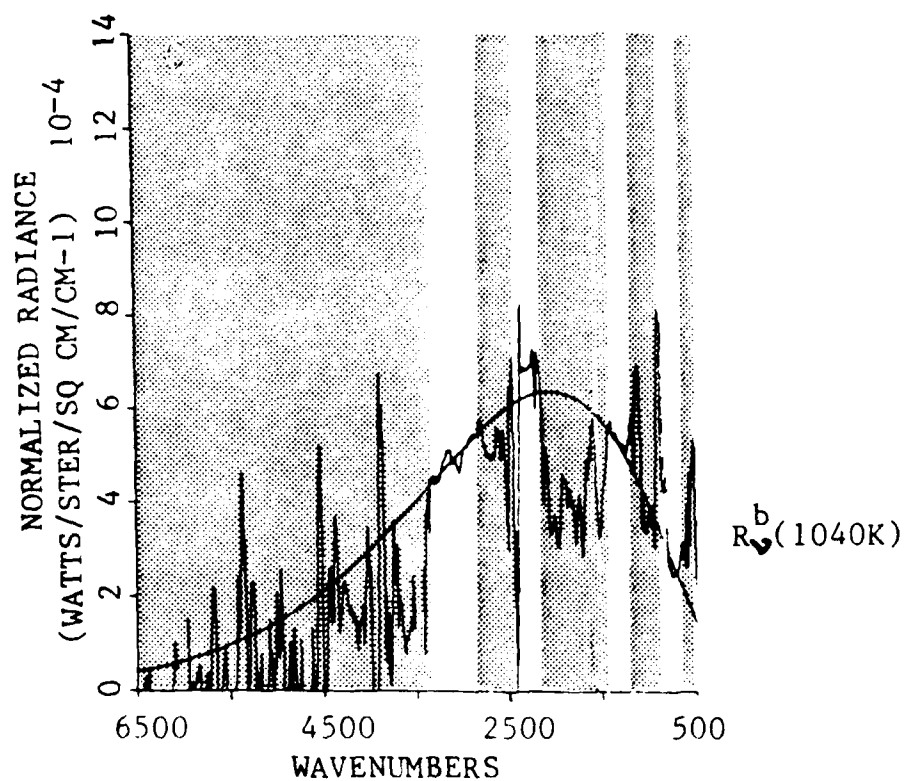
Figure 71. Normalized Emission Spectrum of Butane Pyrolysis (1100°C, 66 cm Reaction Distance). Theoretical Black-Body Curve Corresponds to 1040 K.

thermocouple measurements of the reactor wall at the optical ports. As expected, the experiments done at the longer reaction distances indicate a gas temperature that is higher than the thermocouple measurements, but that are somewhat lower than the nominal reactor temperature of 1373 K. This is due to the optical section being located outside the heated section of the reactor, which allows the gases to cool.

The model predictions are compared to the measured values in Fig. 72. In general, the agreement was within 20°C. Of course, the agreement between the measured and calculated temperatures is not a complete validation of the model because the fuel temperature as a function of the distance from the injector varies with the injector position and the temperature is measured only at one position in the reactor. However, validation of the model at several different injector positions and more than one reactor temperature (1100, 1300°C) helps to establish confidence in the model.

The model was validated against measurements made for butane pyrolysis experiments at 1100 and 1300°C. Next the heat transfer model was incorporated into the hydrocarbon cracking model as a subroutine which provided an updated average temperature after each time increment. The cracking of butane was modeled fairly well, although the overall rate appeared to be a little fast (Figs. 66 through 68). It was thought that neglect of the endothermic reaction heat may be responsible.

While the heat transfer model was validated against butane pyrolysis. The assumption was that the time-temperature histories is primarily controlled by the mixing of the cold and hot streams, which would be similar for both species and was therefore, used for all the simulations.

The time-temperature profiles from these simulations are shown in Figs. 73 and 74.

Conclusions

The comparisons of the simulations and the experiments show an improvement over previous work in that the model predicts to within a factor of two the correct values for the major species, and with some adjustment of rates, can predict the onset of sooting correctly. More work needs to be done in terms of sensitivity analyses in terms of thermodynamics, important reactions, and kinetics.
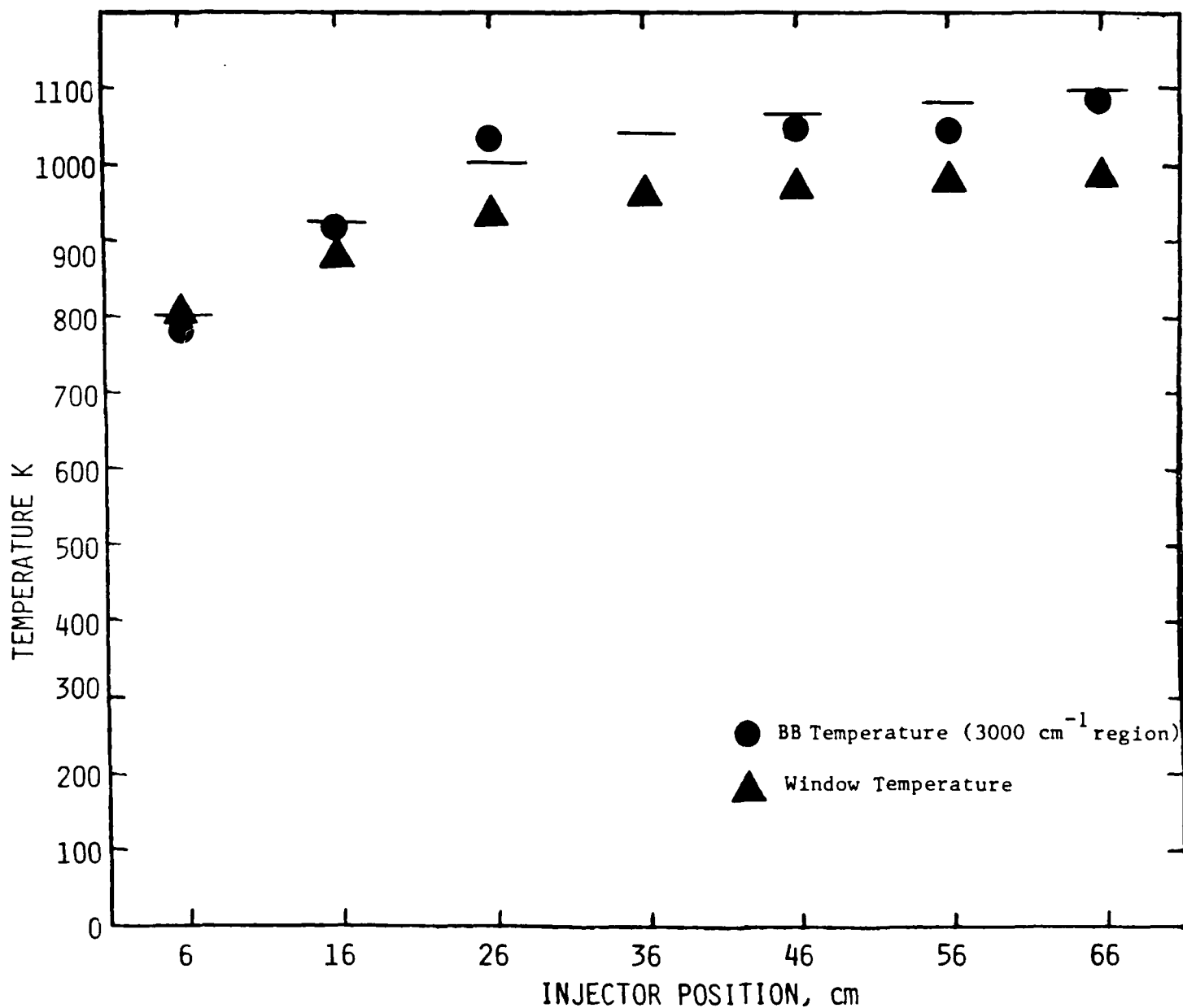
Figure 72. Measured Average Gas Temperatures for the Complete Set of Data of Which Fig. 71 is Part (●) Compared with the Reactor Wall Temperature at Window Height as Measured by a Thermocouple (▲). (——) Predictions of Heat Transfer Model for Average Gas Temperature at Window Height.
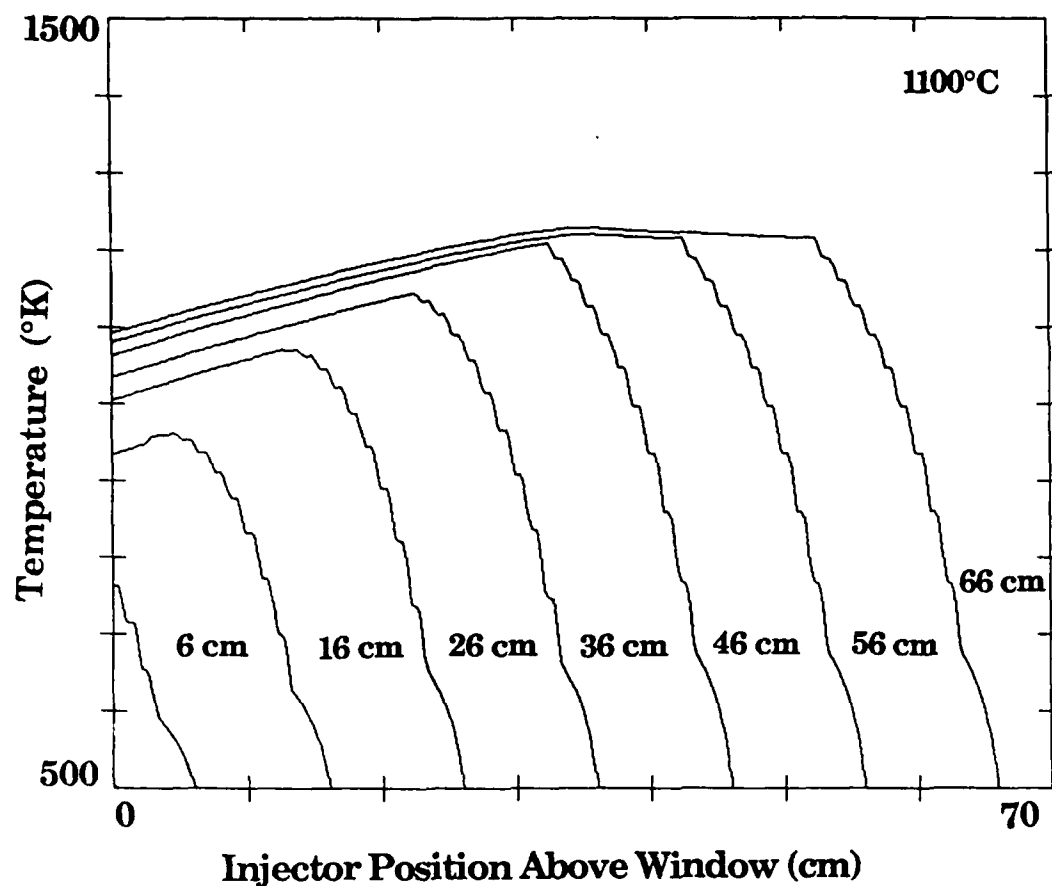
Figure 73. Temperature Simulation for the Entrained Flow Reactor at 1100°C for Butane. The Fuel is Injecting at 20°C (293 K) at the Position Indicated, and Traverses the Reactor, Exiting at 0 cm.
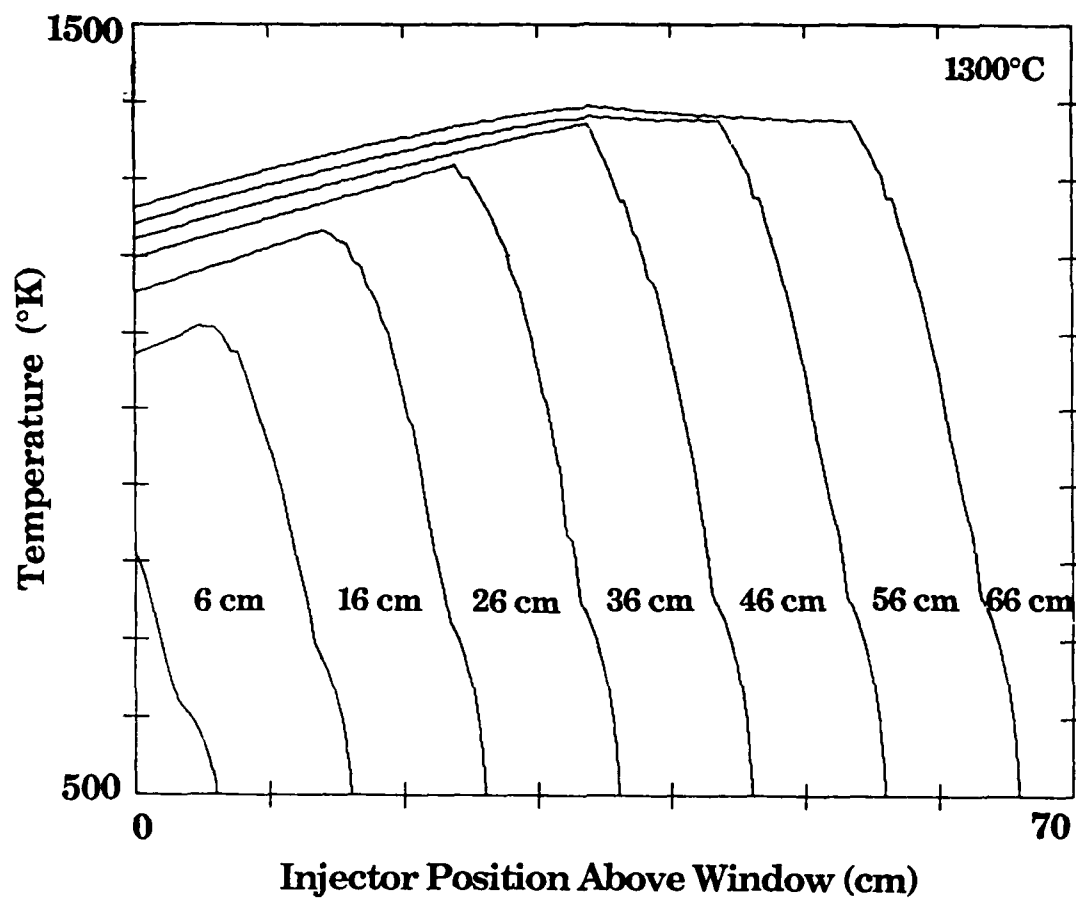
Figure 74. Temperature Simulation for the Entrained Flow Reactor at 1300°C for Butane. The Fuel is Injecting at 20°C (293 K) at the Position Indicated, and Traverses the Reactor, Exiting at 0 cm.

Task V - High Pressure Experiments

A set of pyrolysis experiments was done at high pressure (200 psig) with a selected set of fuels. These experiments were done in a modified version of our heated tube reactor (HTR), discussed in Section II. Originally the experiments were planned for our high pressure entrained flow reactor (HPR), but satisfactory material balances were not achieved in that system which was designed for pyrolysis of solid fuels. To eliminate this problem, the experiments were done in a version of the HTR (see Fig. 8) which included the pressure and flow control system from the HPR (see Fig. 9). The important features of the pressurized HTR are given in Fig. 75. Unfortunately, the maximum operating temperature was limited to 800°C at 200 psig. The residence time at the maximum temperature was about 1.3 s.

The results of experiments with ten fuels are shown in Table 10. All of the product yields are given in weight percent. The condensable products were collected in two locations (refer to Fig. 75); from a U-tube cooled in a water bath and from a Balston filter. The products from both locations were soluble in organic solvents like acetone and were liquid in every case except for tetralin where some solid crystals (probably naphthalene) were found. The yield of products collected on the filter was determined gravimetrically. The yield of products from the U-tube was determined by washing with acetone and analyzing the extract in a capillary GC, using an average FID response factor. The acetone extract from the U-tube and filter housing was filtered and the amount of coke (residue) determined. This was negligible in every case, as expected, since soot formation should be unimportant under these conditions.

The yields of gases were determined by a separate GC system configured as a refinery gas analyzer. This produced a backflush peak which included C_6 hydrocarbons and above. A molecular weight needed to be assumed for this peak to estimate the material balance closure. A value equal to that of the parent hydrocarbon was assumed in each case (see note c in Table 10). The estimated material balances ranged between 80 and 120 percent as indicated by the last column in Table 10. Of course, some of this variability is due to assumptions regarding the GC response factors.

In order to determine the effects of increased pressure, a comparison was made, on a relative basis, of the important gas species yields for the experiments done under pressure with experiments done at one atmosphere pressure, 1300°C reactor temperature, 26 cm reactor distance in the entrained flow reactor (see Appendix A). Under the latter conditions, it was estimated that the fuel reached a maximum temperature of 900°C. Since the reaction severities were not identical in

- 114 -
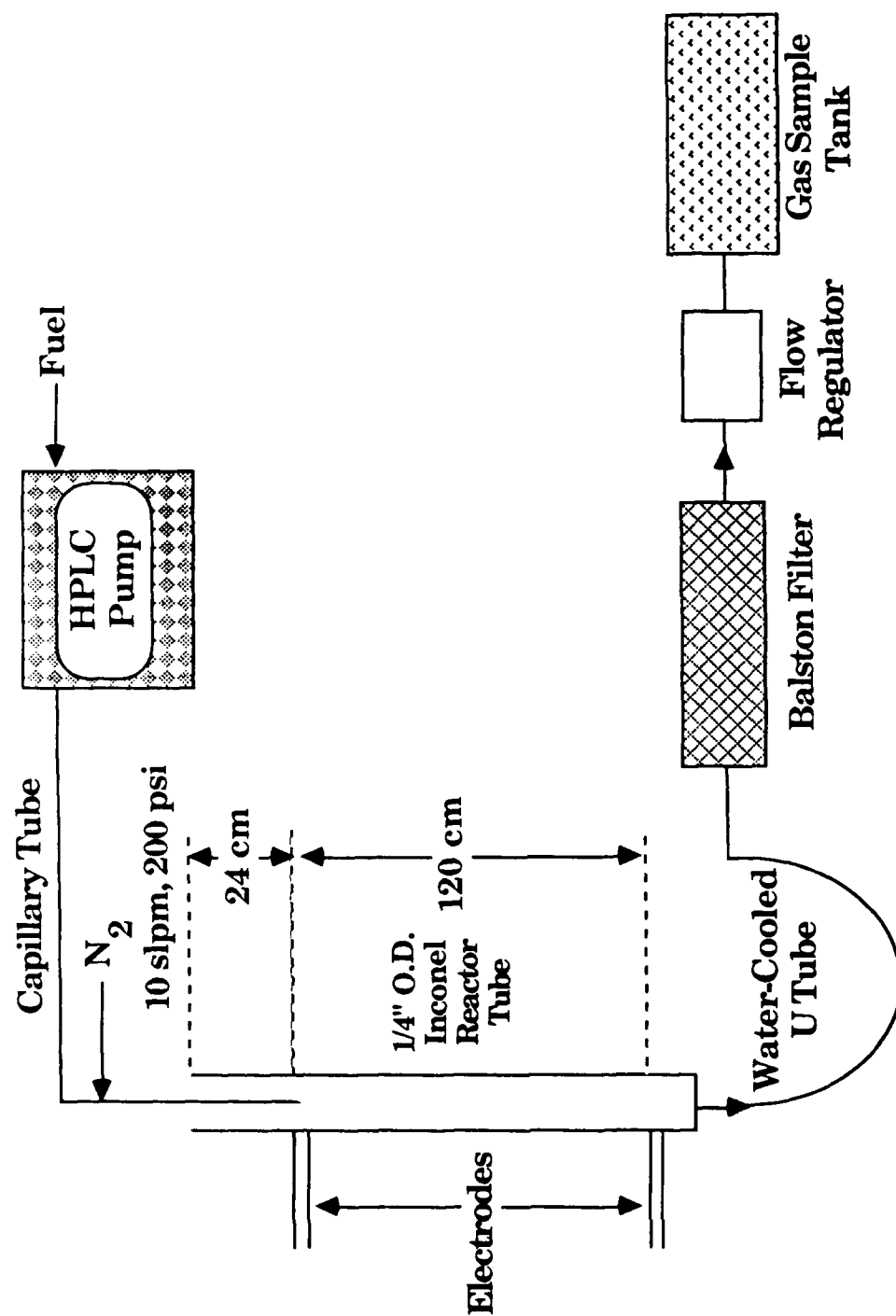
Figure 75. Schematic of Pressurized Heated Tube Reactor.

TABLE 10

SUMMARY OF HIGH PRESSURE PYROLYSIS EXPERIMENTS WITH SEVERAL FUELS

Weight Percent Products

Exp. No.	Fuel	Filter[a]	U Tube[b]	Coke[b]	C_6+/MW[c]	H_2	C_2H_4	C_2H_6	C_2H_2	CH_4	C_3	C_4	C_5	Sum
160	Decalin	10.6	46.2	0	0.182	0.13	5.30	0.45	-	1.24	3.79	2.23	-	95
162	Tetralin	29.2	42.6	0.005	0.032	0.81	2.00	0.44	-	0.59	0.60	0.25	-	81
163	Tetralin	28.1	38.8	0.005	0.041	0.83	1.48	0.15	-	1.21	0.26	0.16	-	77
164	Dodecane	3.6	41.4	0.003	0.035	0.12	15.48	0.73	0.13	2.26	11.18	4.67	-	86
167	JP-8 2383	23.9	14.4	0.051	0.245	0.94	12.36	1.38	0.22	6.77	7.89	6.69	0.26	107
168	JP-8 2398	30.0	12.2	0.084	0.218	0.89	11.09	1.21	0.13	6.17	7.03	5.87	0.26	103
169	JP-8 2414	28.6	43.2	0.136	0.171	0.95	9.62	1.10	0.09	5.58	5.84	3.47	0.26	121
170	JP-8 2429	27.9	19.7	0.136	0.245	1.06	10.18	1.24	0.13	5.38	5.73	5.52	0.13	109
171	JP-4	9.4	14.2	0.005	0.229	0.78	18.73	1.84	0.20	4.64	11.93	8.56	0.75	101
172	JP-7	11.8	26.6	0.005	0.198	0.84	17.62	1.87	0.19	7.02	11.08	8.21	0.63	112
173	XTR	29.5	70.5	0	0.069	0.08	2.38	0.18	-	0.92	1.04	0.68	-	114

NOTES:

a. Products recovered on filter were liquids or soluble solids; yield was determined gravimetrically.

b. U tube (and filter housing) were washed with acetone, filtered to measure coke; capillary GC was used to determine the sum of products (U tube fraction) in the extract.

c. Average MW was assumed to be the same as the parent hydrocarbon for pure fuels. A value of 130 was used for mixed fuels.

CO_2; CO were zero in every case.

the two cases, the comparisons were made based on examining the ratio of the yields of C_2H_6, CH_4 and H_2 to the C_2H_4 yield. These ratios are usually fairly constant over a wide range of conversions in primary hydrocarbon pyrolysis. The calculated ratios are given in Table 11 for fuels which have comparable 1 atm and 15 atm experiments. The hydrocarbon partial pressure ranged from about 0.006 atm in the 1 atm total pressure experiments to about 0.18 atm in the 15 atm total pressure experiments, a factor of 30 increase.

Most of the previous work on effects of pressure on hydrocarbon pyrolysis has been done on linear aliphatic fuels, principally hexadecane. This literature, which is rather sparse, was recently reviewed by Rebick (64). Pressure is known to have a modest effect on the overall rate and a more significant effect on the product selectivity (64). As the hydrocarbon partial pressure increases, the rates of bimolecular reactions, like hydrogen abstraction, increase faster than the rates of unimolecular reactions, like radical decomposition. The result is an increase in the selectivity toward paraffin products relative to olefins. These effects can be predicted by the AFR hydrocarbon cracking model (44) discussed in Section IV, which matches literature data on high pressure (68 atm) pyrolysis of hexadecane as

well as data for 1 atm pyrolysis of Solpar (compare Figs. 64 and 65). For example, increasing pressure would favor the following bimolecular reaction:

$$C_2H_5 \cdot \quad + \; RH \longrightarrow C_2H_6 + R \cdot$$

over these unimolecular decompositions:

$$C_2H_5 \cdot \longrightarrow C_2H_4 + H \cdot$$

$$C_3H_7 \cdot \longrightarrow C_2H_4 + CH_3 \cdot$$
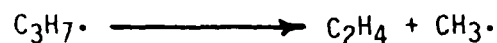
This phenomenon would result in an increase in the yield ratio of ethane to ethylene with increasing pressure. The yield ratios of H_2 and CH_4 would be less affected by pressure since they decrease simultaneously with ethylene.

The results in Table 11 are largely consistent with this scheme, with the exception of dodecane. This is somewhat surprising in light of the fact that this fuel is a linear aliphatic and would be expected to best follow the above reaction steps. The rest of the fuels, except decalin, either contain aromatic components or groups. Most of our understanding of hydrocarbon pyrolysis, in general, and on

TABLE 11

COMPARISON OF GAS PRODUCT YIELD RATIOS FOR EXPERIMENTS AT 1 ATM AND 15 ATM

	$\dfrac{C_2H_6}{C_2H_4}$		$\dfrac{H_2}{C_2H_4}$		$\dfrac{CH_4}{C_2H_4}$	
	1 atm	15 atm	1 atm	15 atm	1 atm	15 atm
Dodecane	0.06	0.05	0.03	0.01	0.24	0.14
Decalin	0.04	0.09	0.07	0.02	0.32	0.23
JP8 2383	0.08	0.11	0.06	0.08	0.41	0.55
JP8 2398	0.09	0.11	0.07	0.08	0.51	0.56
JP8 2429	0.07	0.12	0.08	0.10	0.47	0.53
JP8 2414	0.06	0.11	0.08	0.10	0.44	0.58
Tetralin	0.03	0.17	0.23	0.47	0.49	0.52

pressure effects, in particular, has been developed from work on pure linear aliphatic compounds like dodecane and hexadecane. The effects of pressure on the product distribution appears to be most important for dodecane, decalin, tetralin, JP8 2429 and JP8 2414 fuels, and least important for the JP8 2383 and JP8 2398 fuels.

Task VI - Characterization of Multi-Component Fuel Sprays for Gas Turbine Combustors - (deleted from original contract).

IV. CONCLUSIONS AND RECOMMENDATIONS

During the course of this program, we have achieved a number of significant accomplishments:

- A data base of detailed pyrolysis measurements on a large number of fuels, including several high density, aromatic fuels has been created. Temperature varied from 800°C to 1500°C, pressures from 1 to 15 atm and residence times from 100 ms to 1 sec.

- A key conclusion of Task I is that in almost all cases at one atmosphere the fuels have decomposed to form a limited number of small species prior to the onset of sooting. The aliphatic portion of the fuels formed H_2, C_1's, and C_2's. The aromatic portion of the fuels formed benzene, 2-ring and possibly 3-ring aromatics. This is a significant result and justifies our approach to modeling the sooting tendencies of complex fuels based on a limited number of small species, since the fuels all crack to these starting fragments prior to soot formation.

- The measurements of radiance for these fuels show factors of two or three variation for comparable amounts of soot. The causes of this are probably due to soot age (H/C content) which would change the optical constants for the soot or soot particle size. This observation is significant for heat transfer from the soot in combustion, and for its impact on the soot signature left by an engine.

- In all cases, we find that the addition of small amounts of hydrogen (as H_2) reduces the soot while similar amounts of O_2 increase it. This again has significance for the soot signature of a jet engine. One can imagine adding a pulse H_2 to reduce the IR signature under emergency conditions.

- In Task II, a factor analysis correlation was performed which shows that the complex IR spectra of the hydrocarbon can be characterized by a few (10) factors which can reproduce the spectra to within 5%. Secondly, these factors can be used to predict the combustion properties of the fuels, in particular the sooting as measured in Task I, or the smoke point as measured by standard techniques.

- The hydrocarbon cracking model began in Phase I was extended using a modified Rice-Kossiakoff-Herzfeld (RKH) mechanism. This model predicts the decomposition of long chain aliphatics into small molecules, (C_2H_2, C_2H_4, H_2).

- A soot model based on published free radical mechanisms and rates was implemented on AFR's Sun 3/260 workstation and used to predict the growth of the soot precursors from the small molecules produced.

- A heat transfer model was developed to provide the temperature-time profiles required by both models.

- The combination of these models can predict not only the soot, but also the intermediate light species of pyrolysis (C_2's, C_3's, C_4's, light aromatics) to within a factor of two.

There remain a number of unanswered questions and areas where more work should be done.

1) The emission/transmission experiments raise a number of tantalizing questions about the nature of the radiating soot. Mie theory calculations should be performed to attempt to correlate the experimental observations of Task I with the optical constants and the size parameter for the particles.

2) More emission/transmission experiments should be performed to investigate the effect of added H_2 on the optical constants and the radiance.

3) In order to investigate the potential for a model which would predict the yield of primary pyrolysis products (H_2, C_1's, and C_2's), correlations should be sought for these species with the FT-IR liquid cell spectra. This would be done using the existing database for Task I. Such a predictive model could be developed from AFR's similar model for coal pyrolysis.

4) In the soot modeling, substantial work should be done to investigate the sensitivity of the model to thermodynamics, reaction kinetics, and to test which reactions are significant. The model should also be tested against literature data.

5) The soot model should be extended beyond acenaphthalene.

6) The three models, hydrocarbon cracking, soot growth, and heat transfer
   should be integrated to provide a significant predictive capability.

7) The high pressure work was limited due to experimental difficulties with
   mass balances. An effort should be made to rectify these problems and
   obtain data at elevated temperatures and pressures.

8) Pressure effects on the pyrolysis product distributions were shown to be
   important for all of the pure fuels examined, and two of the four multi-
   component jet fuels. However, only one series of multi-component fuels
   (JP8) was examined. Additional work on other multi-component fuels is
   recommended.

9) To date, the examination of pressure effects on hydrocarbon pyrolysis has
   been restricted to studies on primary pyrolysis. Additional studies are
   needed for a wide range of fuels which can assess the impact of pressure on
   secondary pyrolysis and soot formation.

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APPENDIX A

Product Summaries from Entrained Flow Reactor
Mass Balance Experiments

TABLE A-1

RUN CONDITIONS

2490.50 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid.
763.120 mm. Final Pressure for 86.7060 liters

UTRC 2A
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	42.5697
Tar	6.25175
Gas	37.8807
Water	1.34835
Missing	11.9494

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	9.44388	.40622	7.98291	2.36897	0
CO	3.95199	.09709	1.65096	0	2.20103
Hydrogen	7.50853	2.58543	0	7.50053	0
CO2	.25097	3.95122E-3	.07002	0	.18557
Acetylene	10.7246	.29112	9.89996	.82472	0
Ethylene	1.32871	3.34925E-2	1.13884	.18987	0
Ethane	2.25909E-4	5.31479E-6	1.80727E-4	4.51818E-5	0
Propylene	.06782	1.46244E-3	.07459	1.24361E-2	0
Benzene	2.45733	2.17528E-2	2.26836	.18896	0
Paraffins	.45394	3.81413E-3	.38907	.06486	0
Olefins	1.86814	1.56965E-2	1.69118	.26695	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	1.34835	3.66018E-2	0	.14980	1.19854
Other	0	99.1486	0	0	0
Gas Total:	39.2290	100	24.1761	11.5671	3.58647

TABLE A-2

RUN CONDITIONS

2992 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
758 mm. Final Pressure for 96.3400 liters

Gas Scans =>	0 - 0 - 76	0 : 0	
Analysis =>	9 - 19 - 86	14 : 18	
Stored =>	9 - 19 - 86	14 : 31	

ERBLS 1
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	42.3462
Tar	6.21657
Gas	45.9389
Water	5.03617E-2
Missing	5.44786

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	9.25802	.26385	6.94351	2.31450	0
CO	3.31179	.09071	1.41943	0	1.89235
Hydrogen	7.82085	2.91029	0	7.82085	0
CO2	.17713	2.99472E-3	4.83058E-2	0	.12883
Acetylene	11.5975	.33245	10.7057	.89185	0
Ethylene	1.45905	3.99673E-2	1.25055	.20849	0
Ethane	2.06156E-4	5.27068E-6	1.64925E-4	4.12312E-5	0
Propylene	.10032	1.83219E-3	.08599	1.43370E-2	0
Benzene	10.1748	.10005	9.39238	.78244	0
Paraffins	.12692	1.15891E-3	.10878	1.81372E-2	0
Olefins	1.91449	1.74810E-2	1.64091	.27358	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	5.03617E-2	1.48565E-3	0	5.59518E-3	4.47665E-2
Other	0	99.2480	0	0	0
Gas Total:	45.9893	100	31.5957	12.3298	2.06595

A-4

TABLE A-3

RUN CONDITIONS

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 9 - 10 - 86   15 : 47
Stored => 1 - 1 - 80   2 : 10

2969.60 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
765 mm. Final Pressure for 95.3766 liters

UTRC 7A
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	45.2586
Tar	6.22929
Gas	39.6264
Water	1.35547
Missing	7.52963

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	5.08486	.23660	3.91364	1.27121	0
CO	3.98206	.10345	1.62956	0	2.17249
Hydrogen	8.25026	3.08496	0	8.25026	0
CO2	.12679	3.00653E-3	4.82113E-2	0	.12858
Acetylene	10.2707	.29542	9.48092	.78992	0
Ethylene	.95080	2.58722E-2	.81493	.13587	0
Ethane	2.28925E-3	5.51891E-5	1.76740E-3	4.41851E-4	0
Propylene	-1.94233E-4	-3.34210E-6	-1.57986E-4	-2.65269E-5	0
Benzene	9.22956	.89503	8.98136	.74820	0
Paraffins	.31357	2.84417E-3	.26876	4.48092E-2	0
Olefins	1.04933	9.51780E-3	.89938	.14995	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	1.35547	3.97207E-2	0	.15059	1.20487
Other	0	99.3854	0	0	0
Gas Total:	40.9819	100	25.9384	11.5411	3.50595

TABLE A-4

RUN CONDITIONS

Gas Scans =) 8 - 8 - 76   0 : 0
Analysis =) 5 - 27 - 86   17 : 45
Stored =) 9 - 25 - 86   12 : 42

1632 mg. DEGAS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 90.5596 liters

JP7
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	36.3970
Tar	7.40196
Gas	50.6080
Water	6.26819
Missing	-.67530

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	5.57190	.15571	4.17892	1.39297	0
CO	6.91485	.11042	2.96370	0	3.95114
Hydrogen	0	0	0	0	0
CO2	1.04458	1.06163E-2	.28488	0	.75430
Acetylene	19.1384	.31193	15.7435	1.39484	0
Ethylene	.36173	1.49493E-2	.80236	.13377	0
Ethane	2.22835E-4	4.14102E-6	2.22268E-4	5.55571E-5	0
Propylene	2.25802E-3	2.40391E-5	1.93534E-3	3.22571E-4	0
Benzene	16.1414	.09253	14.9002	1.24128	0
Paraffins	0	0	0	0	0
Olefins	.70814	3.72692E-3	.60009	.10005	0
HCN	.96913	1.60495E-2	.43068	3.58581E-2	0
Ammonia	6.98756E-3	1.83788E-4	0	1.23330E-3	0
COS	-6.46050E-3	-4.81455E-5	-1.29210E-3	0	-1.72301E-3
CS2	.16631	9.78466E-4	2.62603E-2	0	0
SO2	2.19291E-2	1.53208E-4	0	0	1.09645E-2
Water	6.26819	.10779	0	.69639	5.57179
Other	0	99.1749	0	0	0
Gas Total:	56.8762	100	40.9315	4.99629	10.2919

TABLE A-5

RUN CONDITIONS

Gas Scans => 8 - 8 - 76   0 : 0
Analysis => 9 - 18 - 86   15 : 12
Stored => 9 - 18 - 86   7 : 57

3084 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
765.800 mm. Final Pressure for 90.5596 liters

JP4-S
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	25.5892
Tar	7.08055
Gas	55.0966
Water	9.92187E-3
Missing	12.2237

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	5.27430	.33690	5.08072	1.69357	0
CO	3.74658	.18849	1.60526	0	2.14076
Nitrogen	6.92070	2.37618	0	6.92070	0
CO2	.57283	1.85567E-2	.15621	0	.41661
Acetylene	16.6049	.51786	15.3279	1.27691	0
Ethylene	3.26351	.09451	2.79716	.46635	0
Ethane	6.95152E-4	1.87894E-5	5.56122E-4	1.39030E-4	0
Propylene	.19671	3.79798E-3	.16860	2.81111E-2	0
Benzene	11.8214	.12289	10.9123	.90907	0
Paraffins	.36142	3.48895E-3	.30977	5.16476E-2	0
Olefins	4.82534	4.65806E-2	4.13580	.68954	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	9.92197E-3	3.09439E-4	0	1.10232E-3	8.81955E-3
Other	0	98.7979	0	0	0
Gas Total:	55.1065	100	40.4949	12.0871	2.56620

A-7

PYROLYSIS SUMMARY REPORT   USARUN 92

RUN CONDITIONS

1463 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
755 mm. Final Pressure for 92.4864 liters

Gas Scans =>	0 - 0 - 76		0 : 0		
Analysis =>	5 - 23 - 86		14 : 10		
Stored =>	9 - 25 - 86		12 : 59		

JP4
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	34.5639
Tar	5.43403
Gas	55.0107
Water	8.18820
Missing	-3.19685

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	5.93790	.14507	4.45342	1.48447	0
CO	7.28118	.10165	3.12071	0	4.16046
Hydrogen	4.56596	.86887	0	4.56596	0
CO2	1.61592	1.43563E-2	.44066	0	1.17526
Acetylene	14.6439	.22017	13.5178	1.12612	0
Ethylene	1.20707	1.68519E-2	1.03458	.17249	0
Ethane	5.24073E-4	6.82883E-6	4.19258E-4	1.04814E-4	0
Propylene	5.88639E-3	5.47867E-5	5.04523E-3	8.41166E-4	0
Benzene	18.1681	.08874	16.7710	1.39713	0
Paraffins	2.97268E-2	1.38339E-4	2.54789E-2	4.24792E-3	0
Olefins	1.15575	5.37852E-3	.99060	.16515	0
HCN	.80993	1.17263E-2	.35993	2.99675E-2	0
Ammonia	1.91610E-3	4.40600E-5	0	3.38192E-4	0
COS	-6.82993E-3	-4.44979E-5	-1.36598E-3	0	-1.82154E-3
CS2	.22404	1.15240E-3	3.53773E-2	0	0
SO2	2.10890E-2	1.28810E-4	0	0	1.05445E-2
Water	8.18820	.12310	0	.90970	7.27849
Other	0	99.2283	0	0	0
Gas Total:	63.1989	100	40.7537	9.85654	12.6229

TABLE A-7

Gas Volas =   Ø - Ø - 76   Ø : Ø
Analysis => 9 - 11 - 86   7 : 16
Stored => 9 - 12 - 86   15 : 48

RUN CONDITIONS

2762.30 mg. DEOX COAL
Ø sec. Ø Ø Amps
Ø sec. Ø Ø Amps
1500 degrees c. Ø Ø torr with ALTUBE grid
757 mm. Final Pressure for 72.4864 liters

DF2
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	47.5038
Tar	2.37121
Gas	43.3020
Water	1.50223
Missing	5.32856

	wt %	Volume %	%C	%H	%O
Methane	4.2718Ø	.19154	3.20385	1.06795	Ø
CO	3.8722?	.10215	1.55987	Ø	2.21290
Hydrogen	8.8332?	3.15984	Ø	8.9332?	Ø
CO2	.40146	6.73910E-3	.18948	Ø	.29178
Acetylene	14.5616	.48422	13.5342	1.12748	Ø
Ethylene	1.01125	2.5578 E-2	.9...	.14452	Ø
... ne	5.05...4	1.33565E-5	4.44084E-4	1.11825E-4	Ø
Propylene	.76879	1.77256E-3	.08639	1.44039E-2	Ø
Benzene	7.06631	.08584	8.36911	.69719	Ø
Paraffins	Ø	Ø	Ø	Ø	Ø
Olefins	1.09311	9.61143E-3	.93590	.15620	Ø
HCN	.65224	2.33268E-2	.37895	3.15514E-2	Ø
Ammonia	5.01230E-3	2.17766E-4	Ø	8.84671E-4	Ø
COS	-4.50947E-3	-5.55108E-5	-9.01895E-4	Ø	-1.20267E-3
CS2	.10568	1.02704E-3	1.668/0E-2	Ø	Ø
SO2	1.79289E-2	2.06908E-4	Ø	Ø	8.96449E-3
Water	1.50223	4.26745E-2	Ø	.16689	1.33534
Other	Ø	99.2335	Ø	Ø	Ø
Gas Totals	44.8???	100	29.162??	11.748?	4.?1?49

TABLE A-8

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 9 - 10 - 86   14 : 34
Stored => 9 - 17 - 86   14 : 13

RUN CONDITIONS

2816 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
754 mm. Final Pressure for 90.5596 liters

AFAPL 6
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

          Dry Wt. %

Char   46.6193
Tar   3.05042
Gas   49.4433
Water   .45721
Missing   .42968

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	4.76190	.22751	3.57142	1.19047	0
CO	4.23757	.11569	1.81626	0	2.42140
Hydrogen	7.43587	3.18471	0	7.43587	0
CO2	2.73457E-4	4.75138E-6	7.45717E-5	0	1.99050E-4
Acetylene	14.4176	.41423	13.3095	1.10871	0
Ethylene	1.74489	5.14957E-2	1.53199	.21229	0
Ethane	3.40749E-3	1.39323E-4	4.35717E-3	1.09747E-3	0
Propylene	.21902	5.78047E-3	.18772	3.12979E-2	0
Benzene	13.5482	.13270	12.4978	1.04124	0
Paraffins	.26187	2.38326E-3	.22445	3.74221E-2	0
Olefins	2.71054	2.46688E-2	2.32329	.38735	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	.45721	0	0	5.07960E-2	.40641
Other	0	99.1435	0	0	0
	---------	---------			
Gas Total:	49.9005	100	35.5675	11.5565	2.82801

TABLE A-9

Gas Scans #: 0 - 0 - 76   0 : 0
Analysis #: 9 - 10 - 85   14 : 52
Stored #: 9 - 17 - 86   14 : 2

RUN CONDITIONS

2855 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
763 mm. Final Pressure for 94.4130 liters

AFAPL 2
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

Wt. %

Char	32.0595
Tar	2.94045
Gas	43.3933
Water	.33694
Missing	16.2597

GAS COMPOSITION

	Gas Wt. %	Volume %	XC	XH	XO
Methane	13.4318	.34639	4.07180	1.35726	0
CO	3.14932	.10629	1.71372	0	2.28469
Hydrogen	8.23117	2.78951	0	8.23117	0
CO2	.24518	.13499	.06686	0	.17932
Acetylene	13.6444	.35255	11.6721	.97236	0
Ethylene	1.39230	3.69617E-2	1.19162	.19867	0
Ethane	8.22422E-5	2.04067E-6	6.57938E-5	1.64484E-5	0
Propylene	.13711	2.43018E-3	.11752	1.95938E-2	0
Benzene	9.43164	.09001	8.70634	.72529	0
Paraffins	.09134	8.09478E-4	.07829	1.30531E-2	0
Olefins	1.80197	1.59687E-2	1.54447	.25750	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	.33694	9.64697E-3	0	3.74350E-2	.29951
Other	0	99.1582	0	0	0
	---------	---------			
Gas Total:	43.7302	100	29.1628	11.8123	2.76253

TABLE A-10

RUN CONDITIONS

2731.40 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
763 mm. Final Pressure for 94.4132 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 9 - 10 - 86   10 : 10
Stored => 1 - 1 - 80   2 : 4

UTRC 3B
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	41.9382
Tar	4.94984
Gas	36.9187
Water	.95921
Missing	15.2339

GAS COMPOSITION
------ ---------

	Dry Wt. %	Volume %	%C	%H	%O
Methane	4.66061	.20707	3.49546	1.16515	0
CO	3.86518	.09798	1.65661	0	2.20856
Hydrogen	9.09108	2.80511	0	8.09108	0
CO2	.74629	1.29391E-2	.23351	0	.54279
Acetylene	5.97739	.16045	5.42541	.45197	0
Ethylene	.96431	2.44452E-2	.82651	.13780	0
Ethane	2.66690E-4	6.30990E-6	2.13353E-4	5.33384E-5	0
Propylene	.11270	1.90498E-3	.09661	1.51078E-2	0
Benzene	11.3700	.18346	10.4957	.87436	0
Paraffins	.11523	9.73732E-4	.09876	1.64671E-2	0
Olefins	1.19608	9.34633E-3	.94802	.15895	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	.95921	3.69593E-2	0	.10656	.85264
Other	0	-7719.21	0	0	0
Gas Total:	37.8780	100	23.2468	11.0176	3.60399

TABLE A-11

PYROLYSIS SUMMARY REPORT   -   USARDA 122

RUN CONDITIONS

26.72 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
759.630 mm. Final Pressure for 76.3400 liters

Gas Conns =   0 - 0 - 76   9 : 0
Analysis = 8 - 22 - 86   13 : 30
Stored =.   9 - 15 - 86   11 : 28

UTRC 8A
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

            Dry Wt. %

Char   38.0453
Tar   7.02344
Gas   50.0385
Water   .32452
Missing   1.28742

GAS COMPOSITION

	Dry Wt. %	Volume %	CO	CH	CO
Methane	5.45921	.23343	4.87425	1.35415	0
CO	4.25175	.14330	1.39774	0	2.41004
Hydrogen	15.1833	2.51914	0	1.52710	0
CO2	1.1555	3.02148E-3	5.92492E-2	0	.14425
Acetylene	10.6515	.17452	10.5859	1.03351	0
Ethylene	2.10554	5.02825E-2	1.85451	.31331	0
Ethane	3.25100E-5	9.07921E-7			
Propylene		2.37	.47151	2.00465E-2	0
Propane	14.0530	.12535	13.1615	1.39544	0
Paraffins	.48357	3.98719E-3	.41858	.06979	0
Olefins	3.02023	2.45530E-2	2.58864	.43159	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	.62962	1.66076E-2	0	.06995	.55967
Other	0	98.9235	0	0	0
	----------	---------			
Gas Total:	56.1601	100	40.7170	12.3181	3.11398

TABLE A-12

RUN CONDITIONS

2521 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
758 mm. Final Pressure for 96.3400 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 9 - 19 - 86   13 : 51
Stored => 9 - 19 - 86   14 : 5

ERBLS 2
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	46.3308
Tar	6.02935
Gas	44.5897
Water	1.30470
Missing	1.74533

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	5.95001	.23350	4.46251	1.48750	0
CO	3.70342	.08547	1.58728	0	2.11613
Hydrogen	7.53669	.23746	0	7.53669	0
CO2	.80003	1.17506E-2	.21817	0	.58186
Acetylene	13.0107	.31398	12.0101	1.00052	0
Ethylene	.91264	2.10642E-2	.78222	.13041	0
Ethane	3.15696E-2	7.23150E-4	2.68557E-2	6.71393E-3	0
Propylene	.10298	1.58466E-3	.08827	1.47168E-2	0
Benzene	11.1491	.09237	10.2918	.85737	0
Paraffins	.33567	2.58250E-3	.28770	4.79677E-2	0
Olefins	1.09918	8.45656E-3	.94211	.15707	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	1.30470	3.24295E-2	0	.14495	1.15974
Other	0	99.3863	0	0	0
Gas Total:	45.8944	100	30.6971	11.3839	3.85775

A-14

TABLE A-13

RUN CONDITIONS

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 9 - 17 - 86   15 : 41
Stored => 9 - 17 - 86   16 : 2

3082 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1500 Degrees c. @ 0 torr with ALTUBE grid
754 mm. Final Pressure for 90.5596 liters

UTRC 9A
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

Dry Wt. %

	Dry Wt. %
Char	35.4892
Tar	5.97988
Gas	44.2001
Water	.21906
Missing	13.1116

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	4.74286	.24797	3.55654	1.18551	0
CO	0.07102	.09268	1.40920	0	1.27923
Hydrogen	5.51902	26.9510	0	5.51907	0
CO2	7.124E-4	1.25234E-6	1.14273E-4	0	3.04770E-4
Acetylene	1.20525	.09431	11.5112	.94229	0
Ethylene	1.75125	5.23289E-2	1.50398	.25025	0
Ethane	2.19886E-4	6.13244E-6	1.75909E-4	4.39773E-5	0
Propylene	.06993	1.39316E-3	5.99415E-2	9.99375E-3	0
Benzene	12.8360	.13768	11.8489	.98708	0
Paraffins	.37217	3.70699E-3	.31898	5.31835E-2	0
Olefins	2.52194	2.51195E-2	2.16155	.36038	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	.21906	7.04946E-3	0	2.43381E-2	.19472
Other	0	99.6191	0	0	0
	---------	---------			
Gas Total:	44.4192	100	32.0867	10.4321	1.96587

TABLE A-14

RUN CONDITIONS

2825 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
759 mm. Final Pressure for 90.5596 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 9 - 26 - 86   14 : 14
Stored => 9 - 26 - 86   14 : 34

UTRC 9B
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	44.7858
Tar	4.35398
Gas	46.0999
Water	2.07701
Missing	2.68318

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	6.40033	.30623	4.80025	1.60008	0
CO	4.29915	.11754	1.84261	0	2.45653
Hydrogen	8.61946	3.22661	0	8.61946	0
CO2	.23362	4.00527E-3	.06371	0	.16991
Acetylene	11.5150	.33201	10.6295	.88550	0
Ethylene	1.43828	3.93240E-2	1.23275	.20553	0
Ethane	1.87786E-4	4.79196E-6	1.50229E-4	3.75572E-5	0
Propylene	.10845	1.97684E-3	.09295	1.54982E-2	0
Benzene	11.6814	.11198	10.7831	.89830	0
Paraffins	5.72876E-2	5.22099E-4	4.91012E-2	8.18640E-3	0
Olefins	1.93266	1.76136E-2	1.65648	.27617	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	2.07701	6.11556E-2	0	.23075	1.84625
Other	0	99.1082	0	0	0
Gas Total:	48.1769	100	31.1506	12.7395	4.47270

A-16

TABLE A-15

Gas Scans =>	0 - 0 - 76	0 : 0
Analysis =>	7 - 3 - 87	9 : 6
Stored =>	7 - 7 - 87	18 : 50

RUN CONDITIONS

3330 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 104.047 liters

Tetralin 1300°C
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	1.53153
Tar	33.3633
Gas	24.9661
Water	1.64046
Missing	38.4985

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	2.99611	.14820	2.24708	.74902	0
CO	1.13310	3.20285E-2	.48564	0	.64745
Hydrogen	1.38138	.53236	0	1.38138	0
CO2	4.35872E-4	7.84676E-6	1.18862E-4	0	3.17010E-4
Acetylene	1.50103	3.96042E-2	1.20098	.10004	0
Ethylene	6.11011	.17270	5.23698	.87313	0
Ethane	.19064	5.02945E-3	.15251	3.81283E-2	0
Propylene	.67692	1.27560E-2	.58019	.09673	0
Benzene	10.0669	.10214	9.29277	.77414	0
Paraffins	.70462	6.63903E-3	.60393	.10069	0
Olefins	.39039	6.34081E-3	.33460	5.57867E-2	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	1.64046	4.99366E-2	0	.18225	1.45821
Other	0	99.3258	0	0	0
Gas Total:	26.6066	100	20.1348	4.35133	2.10598

TABLE A-16

RUN CONDITIONS

3450 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
754 mm. Final Pressure for 96.3400 liters

Tetralin 1300°C
Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	34.8985
Tar	14.4347
Gas	28.7342
Water	5.06282
Missing	16.8695

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	2.52173	.13594	1.89130	.63043	0
CO	3.52090	.11254	1.50905	0	2.01184
Hydrogen	4	1.71750	0	4	0
CO2	8.79840E-4	1.78971E-5	2.39932E-4	0	6.39907E-4
Acetylene	3.27536	.10795	3.02348	.25187	0
Ethylene	2.36259	.07552	2.02498	.33761	0
Ethane	4.95154E-3	1.47724E-4	3.96123E-3	9.90309E-4	0
Propylene	.19082	4.06654E-3	.16355	2.72693E-2	0
Benzene	8.59438	.09861	7.93347	.66090	0
Paraffins	.18675	1.98982E-3	.16006	2.66866E-2	0
Olefins	4.05144	4.31681E-2	3.47249	.57895	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	5.06282	.17428	0	.56248	4.50034
Other	0	99.1855	0	0	0
Gas Total:	33.7971	100	20.1826	7.07721	6.51283

A-18

PYROLYSIS SUMMARY REPORT - USARUN 180

RUN CONDITIONS
- - - - - - - - - - - - - -

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 7 - 22 - 87   17 : 18
Stored => 7 - 7 - 87   17 : 50

3610 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
754 mm. Final Pressure for 95.3760 liters

Tetralin 1300°C
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
- -

	Dry Wt. %
Char	61.5235
Tar	3.79501
Gas	25.1499
Water	3.02178
Missing	6.50969

GAS COMPOSITION
- - - - - - - - - - - - - -

	Dry Wt. %	Volume %	%C	%H	%O
Methane	2.90161	.17127	2.17621	.72540	0
CO	2.76220	.09316	1.18388	0	1.57832
Hydrogen	5.98337	2.71618	0	5.98337	0
CO2	.24930	3.97877E-3	.06798	0	.18132
Acetylene	2.69724	.09797	2.48982	.20741	0
Ethylene	.52174	1.75982E-2	.44718	.07455	0
Ethane	3.53602E-3	1.11317E-4	2.82882E-3	7.07205E-4	0
Propylene	4.62900E-2	1.04089E-3	3.96751E-2	6.61484E-3	0
Benzene	8.44445	.10224	7.79507	.64937	0
Paraffins	3.13813E-2	3.52826E-4	2.68969E-2	4.48439E-3	0
Olefins	.75708	8.51201E-3	.64889	.10818	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	3.02178	.10976	0	.33572	2.68606
Other	0	99.3752	0	0	0
Gas Total:	28.1717	100	14.0784	8.09585	4.44571

TABLE A-18

RUN CONDITIONS

Gas Scans =>	0 - 0 - 26 0 : 0
Analysis =>	9 - 11 - 86 7 : 35
Stored =>	7 - 15 - 87 4 : 5

3424.90 mg. DEOX COAL
0 sec. 0 0 Amps
0 sec. 0 0 Amps
1300 Degrees c. 0 0 torr with ALTUBE grid
762.320 mm. Final Pressure for 90.5596 liters

Tetralin 1300°C
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	67.7976
Tar	2.59861
Gas	20.1932
Water	4.08771E-2
Missing	9.36961

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	1.64553	.09551	1.23415	.41138	0
CO	2.35108	.07798	1.00767	0	1.34341
Hydrogen	6.65712	3.81579	0	6.65712	0
CO2	.09635	1.96767E-3	2.62755E-2	0	.07007
Acetylene	3.00738	.10494	2.77611	.23126	0
Ethylene	.19029	6.31163E-3	.16309	2.71925E-2	0
Ethane	2.88595E-4	8.93408E-6	2.30876E-4	5.77190E-5	0
Propylene	4.81262E-2	1.06417E-3	4.12498E-2	6.87224E-3	0
Benzene	5.39794	.06427	4.98284	.41510	0
Paraffins	.20171	2.23019E-3	.17289	2.88252E-2	0
Olefins	.23021	2.54526E-3	.19731	3.28974E-2	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	4.08771E-2	1.44296E-3	0	4.54144E-3	3.63356E-2
Other	0	-7723.09	0	0	0
Gas Total:	20.2341	100	10.6018	7.81527	1.44982

RUN CONDITIONS

3155.50 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with AL TUBE grid
756 mm. Final Pressure for 92.4864 liters

XTB
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	66.8198
Tar	2.72001
Gas	25.1624
Water	.24393
Missing	5.05371

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	2.66542	.13936	1.99906	.66635	0
CO	2.87420	.08587	1.23188	0	1.64231
Hydrogen	7.30153	2.98955	0	7.30153	0
CO2	7.00683E-5	1.33223E-6	1.918?6E-5	0	5.09607E-5
Acetylene	4.59958	.14203	4.16279	.34678	0
Ethylene	.25141	7.51176E-3	.21548	3.59258E-2	0
Ethane	2.26355E-4	6.31166E-6	1.81068E-4	4.525 9E-5	0
Propylene	-9.56577E-3	-1.92594E-4	-8.28727E-3	-1.331o E-3	0
Benzene	7.44861	.07989	6.87581	.57279	0
Paraffins	.08731	8.69635E-4	.07484	1.24777E-2	0
Olefins	.26598	2.64906E-3	.22797	3.80094E-2	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	.24393	7.84901E-3	0	2.71012E-2	.21683
Other	0	99.5764	0	0	0
Gas Total:	25.4064	100	14.7797	8.99965	1.85920

TABLE A-20

	Gas Scans =>	0 - 0 - 76	0 : 0
RUN CONDITIONS	Analysis =>	8 - 13 - 86	13 : 59
	Stored =>	9 - 18 - 86	8 : 17

3206 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
764.300 mm. Final Pressure for 96.3400 liters

BLS
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	64.1609
Tar	2.48908
Gas	28.6844
Water	.47649
Missing	4.18902

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	2.83920	.14463	2.12940	.70980	0
CO	3.02261	.08799	1.29549	0	1.72712
Hydrogen	8.45290	3.37040	0	8.45290	0
CO2	.16748	3.19253E-3	4.56725E-2	0	.12181
Acetylene	7.11702	.22311	6.56972	.54729	0
Ethylene	.35861	1.04392E-2	.30736	5.12462E-2	0
Ethane	2.23344E-2	6.06809E-4	1.78675E-2	4.46688E-3	0
Propylene	-4.15713E-3	-8.06758E-5	-3.56307E-3	-5.94054E-4	0
Benzene	6.30467	.06588	5.81984	.48482	0
Paraffins	.16815	1.63169E-3	.14412	2.40299E-2	0
Olefins	.22808	2.21316E-3	.19549	3.25932E-2	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	.47649	2.74761E-3	0	5.29388E-2	.42355
Other	0	99.4328	0	0	0
Gas Total:	29.1609	100	16.5214	10.3595	2.27249

TABLE A-21

RUN CONDITIONS

Gas Scans => 0 - 1 - 76   0 : 0
Analysis => 8 - 22 - 86   12 : 46
Stored => 9 - 22 - 86   8 : 6

3000 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
758.300 mm. Final Pressure for 94.4130 liters

ERBLS 3
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	59.6100
Tar	1.97000
Gas	31.2737
Water	1.33628
Missing	5.80999

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	6.53333	.31596	4.97500	1.65833	0
CO	3.41113	.09628	1.46203	0	1.94915
Hydrogen	2.39000	3.39047	0	8.89000	0
CO2	.17299	3.03310E-3	4.71770E-2	0	.12582
Acetylene	9.53333	.27957	8.80022	.73311	0
Ethylene	.39454	1.39471E-2	.42387	.07066	0
Ethane	1.00989E-4	2.55559E-6	8.07110E-5	2.01777E-5	0
Propylene	.09026	1.69705E-3	.07736	1.28984E-2	0
Benzene	1.55666	1.51655E-2	1.43695	.11970	0
Paraffins	.13880	1.30483E-3	.11896	1.98347E-2	0
Olefins	.39870	3.74807E-3	.34172	5.69744E-2	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	1.33628	4.05850E-2	0	.14846	1.18782
Other	0	99.4057	0	0	0
Gas Total:	32.6100	100	17.6834	11.7100	3.26280

TABLE A-22

PYROLYSIS SUMMARY REPORT — USARUN 117

RUN CONDITIONS

3216 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
756 mm. Final Pressure for 88.6330 liters

ERBS
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	57.2294
Tar	2.54642
Gas	32.9177
Water	.94415
Missing	6.36815

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	3.63628	.20419	2.72721	.90907	0
CO	3.54133	.11363	1.51781	0	2.02351
Hydrogen	9.43718	4.10899	0	9.43718	0
CO2	.25186	5.02645E-3	.06868	0	.18318
Acetylene	12.5621	.42063	11.5961	.96603	0
Ethylene	.95841	3.07540E-2	.82146	.13695	0
Ethane	3.34111E-5	1.00063E-6	2.67289E-5	6.68222E-6	0
Propylene	.07542	1.61361E-3	.06465	1.07789E-2	0
Benzene	1.07587	1.20370E-2	.99313	.08273	0
Paraffins	.18750	2.00561E-3	.16071	2.67950E-2	0
Olefins	1.19152	1.27447E-2	1.02125	.17026	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	.94415	3.26268E-2	0	.10489	.83925
Other	0	98.9190	0	0	0
Gas Total:	33.8619	100	18.9711	11.8447	3.04596

TABLE A-23

```
                                              Gas Scans => 0 - 0 - 76      0 : 0
RUN CONDITIONS                                Analysis => 7 - 7 - 87     16 : 37
---------------                               Stored => 5 - 22 - 86      26 : 42
 2780 mg. ASIS COAL
 0 sec. @ 0 Amps
 0 sec. @ 0 Amps
 1300 Degrees c. @ 0 torr with ALTUBE grid
 761 mm. Final Pressure for 100.193 liters
```

Decalin 1300°C
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	0
Tar	6.69064
Gas	74.7013
Water	3.35617
Missing	15.2517

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	8.31265	.35460	6.23449	2.07816	0
CO	1.66275	4.05321E-2	.71265	0	.95010
Hydrogen	1.83453	.61235	0	1.83453	0
CO2	8.15249E-4	1.26463E-5	2.22318E-4	0	5.92930E-4
Acetylene	5.78019	.15173	5.33569	.44449	0
Ethylene	26.0143	.63413	22.2969	3.71745	0
Ethane	1.01361	2.30610E-2	.81089	.20272	0
Propylene	6.10523	.09921	5.23279	.87243	0
Benzene	16.1007	.14089	14.8626	1.23815	0
Paraffins	3.59712E-2	6.57030E-4	3.08309E-2	5.14028E-3	0
Olefins	7.76978	.10197	6.65948	1.11030	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	3.35617	.08810	0	.37287	2.98330
Other	0	98.0088	0	0	0
Gas Total:	78.0575	100	62.1766	11.8762	3.93399
```

# TABLE A-24

RUN CONDITIONS
---------------

Gas Scans => 0 - 0 - 76    0 : 0
Analysis => 6 - 18 - 87   10 : 7
Stored => 6 - 18 - 87   14 : 50

3040 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
752 mm. Final Pressure for 101.157 liters

## Decalin 1300°C
## Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

| | Dry Wt. % |
|---|---|
| Char | 5.09868 |
| Tar | 10.2302 |
| Gas | 84.3414 |
| Water | 4.63882 |
| Missing | -4.30921 |

GAS COMPOSITION
---------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 8.55263 | .38603 | 6.41447 | 2.13815 | 0 |
| CO | 4.75263 | .12881 | 2.03912 | 0 | 2.71851 |
| Hydrogen | 4.53947 | 1.63430 | 0 | 4.53947 | 0 |
| CO2 | .24342 | 3.98936E-3 | .06638 | 0 | .17704 |
| Acetylene | 11.8092 | .32845 | 10.9010 | .90812 | 0 |
| Ethylene | 15.3289 | .39494 | 13.1384 | 2.19050 | 0 |
| Ethane | .13157 | 3.05851E-3 | .10526 | 2.63157E-2 | 0 |
| Propylene | 1.67300 | 3.01970E-2 | 1.43393 | .23907 | 0 |
| Benzene | 10.4822 | .10187 | 9.67618 | .80608 | 0 |
| Paraffins | 2.03285 | 1.83461E-2 | 1.74235 | .29049 | 0 |
| Olefins | 24.8585 | .22434 | 21.3062 | 3.55228 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 4.63882 | .13525 | 0 | .51537 | 4.12344 |
| Other | 0 | 97.9633 | 0 | 0 | 0 |
| Gas Total: | 88.9802 | 100 | 66.8234 | 15.2058 | 7.01900 |

A-26

## TABLE A-25

RUN CONDITIONS
----------------

3150 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
754 mm. Final Pressure for 97.3030 liters

Gas Scans =)  0 - 0 - 76    0 : 0
Analysis =)  6 - 30 - 87    0 : 40
Stored =)  7 - 7 - 87    18 : 2

**Decalin 1300°C**
**Injector 56 cm Above Extractor**

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

|  | Dry Wt. % |
|---|---|
| Char | 30 |
| Tar | 5.14285 |
| Gas | 53.1917 |
| Water | 3.82415 |
| Missing | 7.84127 |

GAS COMPOSITION
----------------

|  | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 7.80952 | .37931 | 5.85714 | 1.95238 | 0 |
| CO | 4.82539 | .11697 | 2.06816 | 0 | 2.75723 |
| Hydrogen | 7.98476 | 3.06498 | 0 | 7.98476 | 0 |
| CO2 | .22222 | 3.97877E-3 | 6.06000E-2 | 0 | .16162 |
| Acetylene | 11.3915 | .53819 | 10.4524 | .86909 | 0 |
| Ethylene | 3.54059 | .10145 | 3.03447 | .50592 | 0 |
| Ethane | 1.59127E-2 | 4.25617E-4 | 1.27302E-2 | 3.18255E-3 | 0 |
| Propylene | .25939 | 4.95578E-3 | .22233 | 3.79680E-2 | 0 |
| Benzene | 11.3840 | .11711 | 10.5086 | .87543 | 0 |
| Paraffins | .43584 | 4.16340E-3 | .37356 | 6.22824E-2 | 0 |
| Olefins | 5.51512 | 5.26829E-2 | 4.72701 | .78811 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 3.82415 | .11802 | 0 | .42486 | 3.39928 |
| Other | 0 | 98.7420 | 0 | 0 | 0 |
| Gas Total: | 57.0158 | 100 | 37.2971 | 13.4231 | 6.31814 |

# TABLE A-26

Gas Scans => 0 - 0 - 76     0 : 0
Analysis => 9 - 11 - 86     15 : 59
Stored => 11 - 16 - 87     11 : 33

RUN CONDITIONS
---------------

2855 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
763 mm. Final Pressure for 94.4130 liters


## Decalin 1300°C
## Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
---------------------------------

|  | Dry Wt. % |
| --- | --- |
| Char | 40.3502 |
| Tar | 3.26444 |
| Gas | 52.9098 |
| Water | .47015 |
| Missing | 3.00525 |

GAS COMPOSITION
---------------

|  | Dry Wt. % | Volume % | %C | %H | %O |
| --- | --- | --- | --- | --- | --- |
| Methane | 7.33572 | .34731 | 5.72679 | 1.90893 | 0 |
| CO | 4.35763 | .11584 | 1.86758 | 0 | 2.48995 |
| Hydrogen | 8.2154 | 3.16515 | 0 | 8.22154 | 0 |
| CO2 | 2.81199E-4 | 4.75731E-6 | 7.55828E-5 | 0 | 2.04515E-4 |
| Acetylene | 15.4951 | .37614 | 12.4951 | 1.95700 | 0 |
| Ethylene | 1.95799 | 5.28539E-2 | 1.67619 | .27929 | 0 |
| Ethane | 5.62229E-3 | 1.39505E-4 | 4.49782E-3 | 1.12445E-3 | 0 |
| Propylene | .22522 | 3.99171E-3 | .19303 | 3.21640E-2 | 0 |
| Benzene | 13.9235 | .13282 | 12.8528 | 1.07072 | 0 |
| Paraffins | .26928 | 2.38639E-3 | .23080 | 3.84815E-2 | 0 |
| Olefins | 2.79738 | 2.47012E-2 | 2.38906 | .39831 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | .47015 | 1.34606E-2 | 0 | 5.22340E-2 | .41791 |
| Other | 0 | 99.1423 | 0 | 0 | 0 |
| Gas Total: | 53.3800 | 100 | 37.3911 | 13.5403 | 2.90807 |

## TABLE A-27

RUN CONDITIONS
-----------------

2404 mg. DEOX COAL
0 sec. 0 0 Amps
0 sec. 0 0 Amps
1350 Degrees C. 0 0 torr with ALTURE grid
751 mm. Final Pressure for 94.4130 liters

### JP4-A
### Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-------------------------------

|  | Dry Wt. % |
|---|---|
| Char | 43.5940 |
| Tar | 5.71953 |
| Gas | 47.4469 |
| Water | 1.59627 |
| Missing | 1.64389 |

GAS COMPOSITION

|  | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 5.26295 | .20603 | 3.94722 | 1.31574 | 0 |
| CO | 4.45586 | .09967 | 1.90978 | 0 | 2.54607 |
| Hydrogen | 8.88103 | 2.71222 | 0 | 8.88103 | 0 |
| CO2 | .28702 | 3.94218E-3 | .07927 | 0 | .20875 |
| Acetylene | 13.0199 | .58617 | 12.0187 | 1.00123 | 0 |
| Ethylene | 1.31020 | 2.79844E-2 | 1.14969 | .19151 | 0 |
| Ethane | 5.09209E-4 | 1.07174E-5 | 4.87367E-4 | 1.21841E-4 | 0 |
| Propylene | .07090 | 1.05737E-3 | 6.07694E-2 | 1.01317E-2 | 0 |
| Benzene | 12.3494 | .09916 | 11.3998 | .94967 | 0 |
| Paraffins | .13097 | 9.76635E-4 | .11225 | 1.87163E-2 | 0 |
| Olefins | 1.65340 | 1.23661E-2 | 1.42141 | .23698 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CO2 | 0 | 8.12675E-4 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 1.59627 | 0 | 0 | .17734 | 1.41892 |
| Other | 0 | 99.2061 | 0 | 0 | 0 |
| Gas Total: | 49.0432 | 100 | 32.0974 | 12.7825 | 4.17375 |

## TABLE A-28

PYROLYSIS SUMMARY REPORT  -  USARUN 118

RUN CONDITIONS
----------------

2528 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
764 mm. Final Pressure for 96.3400 liters

### JET A
### Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

|         | Dry Wt. % |
|---------|-----------|
| Char    | 32.5791   |
| Tar     | 6.95896   |
| Gas     | 56.8130   |
| Water   | .74230    |
| Missing | 2.90743   |

GAS COMPOSITION
----------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|-----------|----------|------|------|------|
| Methane   | 6.48167     | .26133     | 4.86125     | 1.62041     | 0 |
| CO        | 4.31954     | .09951     | 1.85135     | 0           | 2.46819 |
| Hydrogen  | 7.95094     | 2.50261    | 0           | 7.95094     | 0 |
| CO2       | .28085      | 4.80523E-3 | .07658      | 0           | .20426 |
| Acetylene | 19.1851     | .46465     | 17.7097     | 1.47533     | 0 |
| Ethylene  | 3.46875     | .07991     | 2.97307     | .49568      | 0 |
| Ethane    | 2.24788E-4  | 4.83371E-6 | 1.79830E-4  | 4.49576E-5  | 0 |
| Propylene | .19850      | 3.04892E-3 | .17013      | 2.83661E-2  | 0 |
| Benzene   | 9.53322     | .07696     | 8.80012     | .73310      | 0 |
| Paraffins | .41299      | 3.17171E-3 | .35397      | 5.90169E-2  | 0 |
| Olefins   | 5.02722     | 3.86079E-2 | 4.30883     | .71839      | 0 |
| HCN       | 0           | 0          | 0           | 0           | 0 |
| Ammonia   | 0           | 0          | 0           | 0           | 0 |
| COS       | 0           | 0          | 0           | 0           | 0 |
| CS2       | 0           | 0          | 0           | 0           | 0 |
| SO2       | 0           | 0          | 0           | 0           | 0 |
| Water     | .74230      | 1.04178E-2 | 0           | .08247      | .65983 |
| Other     | 0           | 98.5868    | 0           | 0           | 0 |
| Gas Total: | 57.5553    | 100        | 41.1053     | 13.1637     | 3.33229 |

# TABLE A-29

Gas Scans => 0 - 0 - 76      0 : 0
Analysis => 9 - 24 - 86      9 : 31
Stored => 9 - 25 - 86      13 : 9

**RUN CONDITIONS**
---------------

31:5 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
754 mm. Final Pressure for 96.3400 liters


**JP5**
**Injector 66 cm Above Extractor**

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

Dry Wt. %
---------

| | Dry Wt. % |
|---|---|
| Char | 39.0112 |
| Tar | 8.37881 |
| Gas | 49.4954 |
| Water | 2.99254 |
| Missing | .12199 |

GAS COMPOSITION
---------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 6.67736 | .32360 | 5.00802 | 1.66934 | 0 |
| CO | 4.29103 | .12240 | 1.83913 | 0 | 2.45190 |
| Hydrogen | 10.0481 | 3.89522 | 0 | 10.0481 | 0 |
| CO2 | .22792 | 4.00530E-3 | 6.21563E-2 | 0 | .16577 |
| Acetylene | 12.5863 | .38420 | 11.5445 | .96173 | 0 |
| Ethylene | 1.70200 | 4.85524E-2 | 1.45878 | .24321 | 0 |
| Ethane | 5.53975E-2 | 1.47495E-3 | 4.43100E-2 | 1.10795E-2 | 0 |
| Propylene | .08760 | 1.66609E-3 | .07508 | 1.25190E-2 | 0 |
| Benzene | 11.4941 | .11770 | 10.6102 | .88390 | 0 |
| Paraffins | .17674 | 1.68065E-3 | .15148 | 2.52569E-2 | 0 |
| Olefins | 2.21946 | 2.11046E-2 | 1.90230 | .31716 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 2.99254 | .09193 | 0 | .33247 | 2.66007 |
| Other | 0 | 98.8317 | 0 | 0 | 0 |
| Gas Total: | 52.4879 | 100 | 32.6961 | 14.5048 | 5.27774 |

A-31

TABLE A-30

RUN CONDITIONS

Gas Scans =>  0 - 0 - 76      0 : 0
Analysis =>  9 - 10 - 86     16 : 20
Stored =>  9 - 25 - 86     13 : 16

2930.90 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
759.300 mm. Final Pressure for 94.4130 liters

## GMSO
## Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

|  | Dry Wt. % |
|---|---|
| Char | 44.3549 |
| Tar | 4.09430 |
| Gas | 48.8053 |
| Water | .15575 |
| Missing | 2.58964 |

GAS COMPOSITION

|  | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 4.52090 | .21625 | 3.39068 | 1.13922 | 0 |
| CO | 4.22051 | .11536 | 1.80891 | 0 | 2.41160 |
| Hydrogen | 8.61510 | 3.33860 | 0 | 8.61510 | 0 |
| CO2 | .35893 | 6.10438E-3 | .09570 | 0 | .25523 |
| Acetylene | 17.2404 | .49519 | 15.9146 | 1.32578 | 0 |
| Ethylene | 1.60079 | 4.37561E-2 | 1.37284 | .22875 | 0 |
| Ethane | 4.47741E-4 | 1.14226E-5 | 3.58192E-4 | 8.95482E-5 | 0 |
| Propylene | .21857 | 3.98309E-3 | .18734 | 3.12349E-2 | 0 |
| Benzene | 9.75044 | .09567 | 9.00063 | .74980 | 0 |
| Paraffins | .25641 | 2.33632E-3 | .21977 | 3.66422E-2 | 0 |
| Olefins | 2.05624 | 1.87351E-2 | 1.76240 | .29383 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | .15575 | 4.58486E-3 | 0 | 1.73042E-2 | .13844 |
| Other | 0 | 99.1942 | 0 | 0 | 0 |
| Gas Total: | 48.9610 | 100 | 33.7525 | 12.4287 | 2.80529 |

A-32

PYROLYSIS SUMMARY REPORT  -  USARUN 108

RUN CONDITIONS
--------------

2922.40 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees C. @ 0 torr with ALTUBE grid
75.? mm. Final Pressure for 96.3400 liters

Gas Scans => 0 - 0 - 76    0 : 0
Analysis => 3 - 5 - 86    13 : 35
Stored => 9 - 15 - 86    15 : 44

## UTRC 1
## Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

|  | Dry Wt. % |
|---|---|
| Char | 24.9599 |
| Tar | 7.22009 |
| Gas | 60.3581 |
| Water | 1.24530 |
| Missing | 6.21646 |

GAS COMPOSITION
---------------

|  | Dry Wt. % | Volume % | %C | %H | %N |
|---|---|---|---|---|---|
| Methane | 12.6353 | 25.453 | 9.42765 | 3.15921 | 0 |
| | 3.15784 | .18600 | 1.70152 | 0 | 2.25842 |
| Hydrogen | 6.51127 | 2.35428 | 0 | 6.51127 | 0 |
| CO2 | .2219.2 | 3.71695E-3 | 5.96465E-2 | 0 | .5937 |
| Acetylene | 1.9244 | .51254 | 16.4527 | 1.27069 | 0 |
| Ethylene | 5.65707 | .15135 | 4.34013 | .80839 | 0 |
| Ethane | 4.75722E-3 | 1.19685E-4 | 3.89736E-3 | 9.51941E-4 | 0 |
| Propylene | .20694 | 5.18607E-3 | .24585 | 4.09897E-2 | 0 |
| Benzene | 3.54160 | 3.30250E-2 | 3.26925 | .27234 | 0 |
| Paraffins | .99058 | 8.81670E-3 | .84903 | .14155 | 0 |
| Olefins | 8.68046 | .07726 | 7.44002 | 1.24043 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 1.24530 | 3.58093E-2 | 0 | .13835 | 1.10695 |
| Other | 0 | 98.5278 | 0 | 0 | 0 |
| Gas Total: | 61.6034 | 100 | 44.3492 | 13.6847 | 3.53446 |

TABLE A-32

|  | Gas Scans => | 0 - 0 - 76 | 0 : 0 |
| RUN CONDITIONS | Analysis => | 6 - 5 - 87 | 11 : 15 |
| --------------- | Stored => | 6 - 11 - 87 | 11 : 20 |

2630 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
756 mm. Final Pressure for 99.2300 liters

## JP8X-2414 (45% aromatic)
## Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-------------------------------

| | Dry Wt. % |
|---|---|
| Char | .23574 |
| Tar | 14.3307 |
| Gas | 98.9110 |
| Water | 1.08891 |
| Missing | -14.5665 |

GAS COMPOSITION
---------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 7.75665 | .30820 | 5.81749 | 1.93916 | 0 |
| CO | 1.04864 | 2.48250E-2 | .44945 | 0 | .59919 |
| Hydrogen | 1.40874 | .44801 | 0 | 1.40874 | 0 |
| CO2 | .41825 | 5.95238E-3 | .11405 | 0 | .30419 |
| Acetylene | 4.60076 | .11296 | 4.24696 | .35379 | 0 |
| Ethylene | 17.5285 | .98015 | 15.0236 | 2.50482 | 0 |
| Ethane | 1.03802 | 2.19576E-2 | .83041 | .20760 | 0 |
| Propylene | 6.63202 | .10466 | 5.68430 | .94771 | 0 |
| Benzene | 14.0217 | .11915 | 12.9434 | 1.07827 | 0 |
| Paraffins | 8.65933 | .06833 | 7.42191 | 1.23741 | 0 |
| Olefins | 35.7827 | .28236 | 30.6693 | 5.11334 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 1.08891 | 2.77611E-2 | 0 | .12097 | .96793 |
| Other | 0 | 98.4667 | 0 | 0 | 0 |
| Gas Total: | 100 | 100 | 83.2011 | 14.9118 | 1.87132 |

A-34

## TABLE A-33

RUN CONDITIONS
----------------

Gas Scans => 0 - 0 - 76     0 : 0
Analysis => 6 - 5 - 87     11 : 1
Stored => 6 - 11 - 87     11 : 11

2410 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
758 mm. Final Pressure for 98.2670 liters

### JP8X-2414 (45% aromatic)
### Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-------------------------------

| | Dry Wt. % |
| --- | --- |
| Char | 24.7717 |
| Tar | 7.46887 |
| Gas | 56.5401 |
| Water | 1.13619 |
| Missing | 10.0829 |

GAS COMPOSITION
---------------

| | Dry Wt. % | | Volume % | %C | %H | %O |
| --- | --- | --- | --- | --- | --- | --- |
| Methane | 9.41908 | | .34696 | 7.06431 | 2.35477 | 0 |
| CO | 4.60580 | | .08443 | 1.97404 | 0 | 2.63175 |
| Hydrogen | 6.34854 | | 1.86543 | 0 | 6.34854 | 0 |
| CO2 | .37544 | | 5.00000E-3 | .10183 | 0 | .27160 |
| Acetylene | 9.25103 | | .22097 | 9.00118 | .74985 | 0 |
| Ethylene | 4.96030 | | .10729 | 4.25147 | .70882 | 0 |
| Ethane | 1.78467E-2 | | 3.60316E-4 | 1.42773E-2 | 3.56934E-3 | 0 |
| Propylene | .34549 | | 4.98235E-3 | .29612 | 4.93707E-2 | 0 |
| Benzene | 12.4836 | | .09693 | 11.5236 | .95998 | 0 |
| Paraffins | .91538 | | 6.60040E-3 | .78457 | .13080 | 0 |
| Olefins | 7.34688 | | 5.29748E-2 | 6.29701 | 1.04987 | 0 |
| HCN | 0 | | 0 | 0 | 0 | 0 |
| Ammonia | 0 | | 0 | 0 | 0 | 0 |
| COS | 0 | | 0 | 0 | 0 | 0 |
| CS2 | 0 | | 0 | 0 | 0 | 0 |
| SO2 | 0 | | 0 | 0 | 0 | 0 |
| Water | 1.13619 | | 2.64682E-2 | 0 | .12623 | 1.00996 |
| Other | 0 | | 99.4850 | 0 | 0 | 0 |
| Gas Total: | 57.6763 | | 100 | 41.3084 | 12.4818 | 3.91332 |

A-35

# TABLE A-34

RUN CONDITIONS
---------------

3076 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
753 mm. Final Pressure for 96.3400 liters

Gas Scans => 0 - 0 - 76     0 : 0
Analysis => 6 - 9 - 87     10 : 35
Stored => 6 - 12 - 87     10 : 21

## JP8X-2414 (45% aromatic)
## Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
--------------------------------

|         | Dry Wt. % |
|---------|-----------|
| Char    | 41.0097   |
| Tar     | 3.32247   |
| Gas     | 46.6102   |
| Water   | 1.33761   |
| Missing | 7.71986   |

GAS COMPOSITION
-----------------

|             | Dry Wt. %    | Volume %     | %C         | %H         | %O       |
|-------------|--------------|--------------|------------|------------|----------|
| Methane     | 7.29641      | .34833       | 5.47231    | 1.82410    | 0        |
| CO          | 3.89573      | .10985       | 1.66971    | 0          | 2.22602  |
| Hydrogen    | 8.50162      | 3.24435      | 0          | 8.50162    | 0        |
| CO2         | .23127       | 3.98406E-3   | .06306     | 0          | .16820   |
| Acetylene   | 9.83713      | .28950       | 9.08065    | .75647     | 0        |
| Ethylene    | 1.71359      | 4.83217E-2   | 1.46872    | .24487     | 0        |
| Ethane      | 1.22696E-2   | 3.22926E-4   | 9.81573E-3 | 2.45393E-3 | 0        |
| Propylene   | .09388       | 1.76491E-3   | .08046     | 1.34156E-2 | 0        |
| Benzene     | 12.3581      | .12509       | 11.4077    | .95033     | 0        |
| Paraffins   | .21836       | 2.05259E-3   | .18716     | 3.12048E-2 | 0        |
| Olefins     | 2.38986      | 2.24639E-2   | 2.04835    | .34151     | 0        |
| HCN         | 0            | 0            | 0          | 0          | 0        |
| Ammonia     | 0            | 0            | 0          | 0          | 0        |
| COS         | 0            | 0            | 0          | 0          | 0        |
| CS2         | 0            | 0            | 0          | 0          | 0        |
| SO2         | 0            | 0            | 0          | 0          | 0        |
| Water       | 1.33761      | 4.06210E-2   | 0          | .14860     | 1.18900  |
| Other       | 0            | 99.1994      | 0          | 0          | 0        |
| Gas Total:  | 47.9478      | 100          | 31.4800    | 12.8146    | 3.58323  |

# TABLE A-35

RUN CONDITIONS
---------------

1900 mq. DEGAS COAL
0 sec. 0 0 Amps
0 sec. 0 0 Amps
1300 Degrees c. 0 0 torr with ALTUBE grid
757 mm. Final Pressure for 88.6330 liters

Gas Scans => 0 - 0 - 76    0 : 0
Analysis => 5 - 29 - 86    11 : 23
Stored => 5 - 29 - 86    14 : 29

## JP8X-2414 (45% aromatic)
## Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-------------------------------

|  | Dry Wt. % |
|---|---|
| Char | 49.6000 |
| Tar | 2.39473 |
| Gas | 27.4058 |
| Water | 7.25208 |
| Missing | 13.3473 |

GAS COMPOSITION
---------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| methane | 3.29844 | .10891 | 2.47383 | .82461 | 0 |
| CO | 4.96054 | .09360 | 2.12608 | 0 | 2.83445 |
| Hydrogen | 4 | 1.02893 | 0 | 4 | 0 |
| CO2 | 1.55329 | 1.86517E-2 | .42358 | 0 | 1.12971 |
| Acetylene | 0.57598 | .13363 | 6.07029 | .50569 | 0 |
| Ethylene | .44118 | 8.32484E-3 | .37813 | .06304 | 0 |
| Ethane | 9.44301E-5 | 1.66305E-6 | 7.55441E-5 | 1.88860E-5 | 0 |
| Propylene | .09877 | 1.24266E-3 | .08466 | 1.41155E-2 | 0 |
| Benzene | 6.03196 | 4.08584E-2 | 5.56810 | .46305 | 0 |
| Paraffins | .11132 | 7.00208E-4 | .09541 | 1.59081E-2 | 0 |
| Olefins | .34737 | 2.18491E-3 | .29773 | 4.96394E-2 | 0 |
| HCN | .30580 | 5.98416E-3 | .13590 | 1.13148E-2 | 0 |
| Ammonia | 6.09209E-3 | 1.89337E-4 | 0 | 1.07525E-3 | 0 |
| COS | -3.80505E-3 | -3.35063E-5 | -7.61010E-4 | 0 | -1.01480E-3 |
| CS2 | .16872 | 1.17298E-3 | 2.66423E-2 | 0 | 0 |
| SO2 | 1.06452E-2 | 8.78808E-5 | 0 | 0 | 5.32262E-3 |
| Water | 7.25208 | .14736 | 0 | .80570 | 6.44638 |
| Other | 0 | 99.4371 | 0 | 0 | 0 |
| Gas Total: | 34.6578 | 100 | 17.6797 | 6.75498 | 10.4148 |

## TABLE A-36

RUN CONDITIONS
----------------

3100 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees C. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 100.194 liters

Gas Scans => 0 - 0 - 76    0 : 0
Analysis => 7 - 3 - 87    8 : 48
Stored => 7 - 7 - 87    18 : 37

JP8X-2383 (20% aromatic)
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-----------------------------

|        | Dry Wt. % |
|--------|-----------|
| Char   | .74193    |
| Tar    | 12.4838   |
| Gas    | 69.6687   |
| Water  | 4.33126   |
| Missing | 12.7741  |

GAS COMPOSITION
----------------

|            | Dry Wt. % | Volume % | %C | %H | %O |
|------------|-----------|----------|----|----|----|
| Methane    | 9.22580   | .42800   | 6.91935 | 2.30645 | 0 |
| CO         | 1.58675   | 4.36482E-2 | .68000 | 0 | .90667 |
| Hydrogen   | 1.29032   | .47688   | 0 | 1.29032 | 0 |
| CO2        | 4.68436E-4 | 8.20000E-6 | 1.27742E-4 | 0 | 3.40694E-4 |
| Acetylene  | 5.47886   | .16289   | 5.07599 | .42286 | 0 |
| Ethylene   | 22.1855   | .61027   | 19.0152 | 3.17031 | 0 |
| Ethane     | 1.67225   | 4.29336E-2 | 1.33780 | .33445 | 0 |
| Propylene  | 6.54838   | .08705   | 5.61262 | .93576 | 0 |
| Benzene    | 14.5264   | .14344   | 13.4093 | 1.11708 | 0 |
| Paraffins  | .16129    | 2.50990E-3 | .13824 | 2.30483E-2 | 0 |
| Olefins    | 6.93548   | .09643   | 5.94440 | .99108 | 0 |
| HCN        | 0         | 0        | 0 | 0 | 0 |
| Ammonia    | 0         | 0        | 0 | 0 | 0 |
| COS        | 0         | 0        | 0 | 0 | 0 |
| CS2        | 0         | 0        | 0 | 0 | 0 |
| SO2        | 0         | 0        | 0 | 0 | 0 |
| Water      | 4.33126   | .12830   | 0 | .48120 | 3.85006 |
| Other      | 0         | 97.7586  | 0 | 0 | 0 |
| Gas Total: | 74        | 100      | 58.1332 | 11.0725 | 4.75707 |

# TABLE A-37

PYROLYSIS SUMMARY REPORT    -    USARUN 15B

| | |
|---|---|
| Gas Scans =) | # - # - 76     # : # |
| Analysis =) | 6 - 5 - 87    1# : 6 |
| Stored =) | 6 - 1# - 87     5 : 8 |

RUN CONDITIONS
--------------

2610 mg. DEOX COAL
# sec. @ # Amps
# sec. @ # Amps
1300 Degrees c. @ # torr with ALTUBE grid
761 mm. Final Pressure for 96.3400 liters

## JP8X-2383 (20% aromatic)
## Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

|  | Dry Wt. % |
|---|---|
| Char | 22.8352 |
| Tar | 5.36398 |
| Gas | 65.0192 |
| Water | .95779 |
| Missing | 5.82375 |

GAS COMPOSITION
---------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 9.92337 | .40341 | 7.44252 | 2.48084 | # |
| CO | 4.63601 | .09395 | 1.98699 | # | 2.64901 |
| Hydrogen | 6.85823 | 2.23127 | # | 6.85823 | # |
| CO2 | .49613 | 6.04467E-3 | .11075 | # | .29537 |
| Acetylene | 11.2260 | .28120 | 10.3627 | .86328 | # |
| Ethylene | 5.62755 | .15394 | 4.82337 | .80417 | # |
| Ethane | 2.51195E-5 | 5.58015E-7 | 2.00956E-5 | 5.02391E-6 | # |
| Propylene | .39274 | 6.31124E-3 | .34091 | 5.68383E-2 | # |
| Benzene | 16.6854 | .14256 | 15.4023 | 1.28311 | # |
| Paraffins | .98273 | 7.79676E-3 | .84230 | .14043 | # |
| Olefins | 8.39519 | .06660 | 7.19552 | 1.19967 | # |
| HCN | # | # | # | # | # |
| Ammonia | # | # | # | # | # |
| COS | # | # | # | # | # |
| CS2 | # | # | # | # | # |
| SO2 | # | # | # | # | # |
| Water | .95779 | 2.45501E-2 | # | .10641 | .85138 |
| Other | # | 99.3726 | # | # | # |
| Gas Total: | 65.9770 | 100 | 48.5075 | 13.7930 | 3.79570 |

PYRREP.000 IS ALREADY OPEN
PYROLYSIS SUMMARY REPORT   -   USARUN 169

RUN CONDITIONS
--------------

3000 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
753 mm. Final Pressure for 97.3030 liters

### JP8X-2383 (20% aromatic)
### Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
--------------------------------

| | Dry Wt. % |
| --- | --- |
| Char | 32.3701 |
| Tar | 3.14935 |
| Gas | 55.0789 |
| Water | 3.39505 |
| Missing | 6.00649 |

GAS COMPOSITION
---------------

| | Dry Wt. % | Volume % | %C | %H | %O |
| --- | --- | --- | --- | --- | --- |
| Methane | 7.95454 | .37715 | 5.96590 | 1.98863 | 0 |
| CO | 4.17002 | .11680 | 1.78727 | 0 | 2.38275 |
| Hydrogen | 8.44155 | 3.21248 | 0 | 8.44155 | 0 |
| CO2 | .23051 | 3.98406E-3 | .06286 | 0 | .16765 |
| Acetylene | 11.5909 | .33864 | 10.6995 | .89134 | 0 |
| Ethylene | 2.47077 | .06593 | 2.11770 | .35307 | 0 |
| Ethane | 5.71280E-2 | 1.49483E-3 | 4.57424E-2 | 1.14356E-2 | 0 |
| Propylene | .25366 | 4.73683E-3 | .21741 | 3.62480E-2 | 0 |
| Benzene | 15.8905 | .15978 | 14.6685 | 1.22198 | 0 |
| Paraffins | .31060 | 2.90007E-3 | .26621 | 4.43849E-2 | 0 |
| Olefins | 3.72418 | 3.47725E-2 | 3.19199 | .53218 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 3.39505 | .10241 | 0 | .37719 | 3.01786 |
| Other | 0 | 98.8817 | 0 | 0 | 0 |
| Gas Total: | 58.4740 | 100 | 39.0232 | 13.8980 | 5.56827 |

PYROLYSIS SUMMARY REPORT  -  USARUN 100

RUN CONDITIONS
---------------

1780 mg. DEGAS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
755 mm. Final Pressure for 90.5596 liters

**JP8X-2383 (20% aromatic)**
**Injector 66 cm Above Extractor**

PYROLYSIS PRODUCT DISTRIBUTION
--------------------------------

|          | Dry Wt. % |
|----------|-----------|
| Char     | 49.4606   |
| Tar      | 1.17415   |
| Gas      | 34.7632   |
| Water    | 4.22106   |
| Missing  | 10.3808   |

GAS COMPOSITION
---------------

|           | Dry Wt. % | Volume % | %C | %H | %O |
|-----------|-----------|----------|-----|-----|-----|
| Methane   | 3.98790   | .12146   | 2.99092 | .99697 | 0 |
| CO        | 5.76070   | .10026   | 2.46903 | 0 | 3.29166 |
| Hydrogen  | 5.80898   | 1.36953  | 0 | 5.80898 | 0 |
| CO2       | .96194    | 1.06546E-2 | .26232 | 0 | .69961 |
| Acetylene | 8.75767   | .16415   | 8.08420 | .67346 | 0 |
| Ethylene  | .50545    | 8.29763E-3 | .43322 | .07222 | 0 |
| Ethane    | 1.96049E-4 | 3.19459E-6 | 1.57319E-4 | 3.93299E-5 | 0 |
| Propylene | .08477    | 9.83719E-4 | .07266 | 1.21145E-2 | 0 |
| Benzene   | 8.60790   | 5.37832E-2 | 7.94595 | .66194 | 0 |
| Paraffins | 0         | 0        | 0 | 0 | 0 |
| Olefins   | .28988    | 1.68186E-3 | .24846 | 4.14245E-2 | 0 |
| HCN       | .51210    | 9.24361E-3 | .22758 | 1.89479E-2 | 0 |
| Ammonia   | 2.95099E-3 | 8.45986E-5 | 0 | 5.20849E-4 | 0 |
| COS       | -4.13223E-3 | -3.35643E-5 | -8.26447E-4 | 0 | -1.10206E-3 |
| CS2       | .11835    | 7.58937E-4 | 1.86877E-2 | 0 | 0 |
| SO2       | 1.48985E-2 | 1.13450E-4 | 0 | 0 | 7.44926E-3 |
| Water     | 4.22106   | .07912   | 0 | .46896 | 3.75210 |
| Other     | 0         | 99.4489  | 0 | 0 | 0 |
| Gas Total: | 38.9842  | 100      | 22.7523 | 8.75561 | 7.74974 |

TABLE A-40

PYROLYSIS SUMMARY REPORT  —  USARUN 183

RUN CONDITIONS
--------------

3350 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 100.194 liters


JP8X-2398 (30% aromatic)
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

|  | Dry Wt. % |
|---|---|
| Char | 1.58208 |
| Tar | 11.3432 |
| Gas | 73.5824 |
| Water | 3.56683 |
| Missing | 10.9253 |

GAS COMPOSITION
---------------

|  | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 7.10447 | .45706 | 6.82835 | 2.27611 | 0 |
| CO | 1.41147 | 4.16801E-2 | .60495 | 0 | .80651 |
| Hydrogen | 1.28358 | .51254 | 0 | 1.28358 | 0 |
| CO2 | .17918 | 3.03830E-3 | 4.88417E-2 | 0 | .13026 |
| Acetylene | 19.0149 | .54557 | 17.5526 | 1.46224 | 0 |
| Ethylene | 17.7256 | .52490 | 15.2355 | 2.54014 | 0 |
| Ethane | 1.58884 | 4.32678E-2 | 1.27043 | .31760 | 0 |
| Propylene | 4.41791 | .08454 | 3.78659 | .63131 | 0 |
| Benzene | 12.6712 | .13431 | 11.6968 | .97441 | 0 |
| Paraffins | .11940 | 2.64200E-4 | .10234 | 1.70626E-2 | 0 |
| Olefins | 4.95522 | .09075 | 4.24712 | .70810 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 3.56683 | .11342 | 0 | .39627 | 3.17056 |
| Other | 0 | 97.9908 | 0 | 0 | 0 |
| Gas Total: | 76.1492 | 100 | 61.3736 | 10.6068 | 4.10734 |

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# TABLE A-41

Gas Scans => 0 - 0 - 76    0 : 0
Analysis => 6 - 5 - 87    10 : 40
Stored => 6 - 11 - 87    11 : 5

RUN CONDITIONS
----------------

2790 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
7599 mm. Final Pressure for 96.3400 liters

## JP8X-2398 (30% aromatic)
## Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-------------------------------

|         | Dry Wt. % |
|---------|-----------|
| Char    | 21.8279   |
| Tar     | 7.16845   |
| Gas     | 59.6989   |
| Water   | 2.59492   |
| Missing | 8.70967   |

GAS COMPOSITION
----------------

|           | Dry Wt. % | Volume %     | %C        | %H          | %O       |
|-----------|-----------|--------------|-----------|-------------|----------|
| methane   | 9.64157   | 4.18476E-2   | 7.23118   | 2.41039     | 0        |
| CO        | 4.51612   | 9.79076E-3   | 1.93561   | 0           | 2.58051  |
| Hydrogen  | 5.73476   | .19923       | 0         | 5.73476     | 0        |
| CO2       | .31541    | 5.00065E-4   | .08601    | 0           | .22939   |
| Acetylene | 9.82078   | 2.63192E-2   | 9.06557   | .75521      | 0        |
| Ethylene  | 6.28642   | 1.50174E-2   | 5.38989   | .89932      | 0        |
| Ethane    | 3.72769E-2| 8.86474E-5   | 2.98215E-2| 7.45539E-3  | 0        |
| Propylene | .42105    | 7.15223E-4   | .36089    | 6.01694E-2  | 0        |
| Benzene   | 13.2211   | 1.20926E-2   | 12.2044   | 1.01670     | 0        |
| Paraffins | .72490    | 6.15672E-4   | .62131    | .10358      | 0        |
| Olefins   | 8.98382   | 7.63007E-3   | 7.70003   | 1.28378     | 0        |
| HCN       | 0         | 0            | 0         | 0           | 0        |
| Ammonia   | 0         | 0            | 0         | 0           | 0        |
| CuS       | 0         | 0            | 0         | 0           | 0        |
| CS2       | 0         | 0            | 0         | 0           | 0        |
| SO2       | 0         | 0            | 0         | 0           | 0        |
| Water     | 2.59492   | 7.12029E-3   | 0         | .28829      | 2.30662  |
| Other     | 0         | 99.9259      | 0         | 0           | 0        |
| Gas Total:| 62.2939   | 100          | 44.6229   | 12.5587     | 5.11654  |

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PYRREP.000 IS ALREADY OPEN

PYROLYSIS SUMMARY REPORT   -   USARUN 16B

RUN CONDITIONS
---------------

3170 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
752 mm. Final Pressure for 96.3400 liters

Gas Scans =>  0 - 0 - 76    0 : 0
Analysis =>  6 - 8 - 87   16 : 37
Stored =>  6 - 9 - 87   10 : 43

## JP8X-2398 (30% aromatic)
## Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

|  | Dry Wt. % |
|---|---|
| Char | 37.0441 |
| Tar | 3.82334 |
| Gas | 52.4757 |
| Water | 3.56208 |
| Missing | 3.09463 |

GAS COMPOSITION
---------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 7.00315 | .34574 | 5.25236 | 1.75078 | 0 |
| CO | 4.18474 | .12201 | 1.79366 | 0 | 2.39127 |
| Hydrogen | 7.44479 | 2.94015 | 0 | 7.44479 | 0 |
| CO2 | .22397 | 3.98936E-3 | 6.10779E-2 | 0 | .16289 |
| Acetylene | 11.4195 | .34707 | 10.5413 | .87816 | 0 |
| Ethylene | 2.56439 | .07476 | 2.19294 | .36645 | 0 |
| Ethane | .10065 | 2.73897E-3 | .08052 | 2.01302E-2 | 0 |
| Propylene | .31307 | 6.08543E-3 | .26833 | 4.47386E-2 | 0 |
| Benzene | 15.2884 | .16001 | 14.1127 | 1.17567 | 0 |
| Paraffins | .27724 | 2.69446E-3 | .23762 | 3.96180E-2 | 0 |
| Olefins | 3.66048 | 3.55753E-2 | 3.13740 | .52308 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 3.56208 | .11184 | 0 | .39574 | 3.16633 |
| Other | 0 | 99.0398 | 0 | 0 | 0 |
| Gas Total: | 56.8378 | 100 | 37.6834 | 12.4791 | 5.72051 |

## TABLE A-43

RUN CONDITIONS
----------------

2790.80 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
766 mm. Final Pressure for 94.4132 liters

Gas Scans => 0 - 0 - 76     0 : 0
Analysis => 9 - 11 - 86     15 : 30
Stored => 9 - 11 - 86     15 : 38

### JP8X-2398 (30% aromatic)
### Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

|        | Dry Wt. % |
|--------|-----------|
| Char   | 45.6929   |
| Tar    | 1.95284   |
| Gas    | 30.1392   |
| Water  | .87688    |
| Missing| 21.3380   |

GAS COMPOSITION
---------------

|           | Dry Wt. %    | Volume %      | %C           | %H          | %O           |
|-----------|--------------|---------------|--------------|-------------|--------------|
| Methane   | 4.82525      | .21785        | 3.61894      | 1.20631     | 0            |
| CO        | 3.67437      | .09479        | 1.57483      | 0           | 2.09953      |
| Hydrogen  | 0            | 0             | 0            | 0           | 0            |
| CO2       | 1.06963E-3   | 1.75613E-5    | 2.91690E-4   | 0           | 7.77949E-4   |
| Acetylene | 5.73306      | .15928        | 5.29219      | .44087      | 0            |
| Ethylene  | 1.03436      | 2.66863E-2    | .88655       | .14781      | 0            |
| Ethane    | 1.86816E-4   | 4.49850E-6    | 1.49453E-4   | 3.73633E-5  | 0            |
| Propylene | .10207       | 1.75571E-3    | .08749       | 1.45868E-2  | 0            |
| Benzene   | 12.4935      | .11570        | 11.5328      | .96075      | 0            |
| Paraffins | .46750       | 4.02046E-3    | .40069       | .06680      | 0            |
| Olefins   | 1.29077      | 1.11005E-2    | 1.10632      | .18445      | 0            |
| HCN       | .43838       | 1.17290E-2    | .19481       | 1.62202E-2  | 0            |
| Ammonia   | 1.09086E-2   | 4.63547E-4    | 0            | 1.92537E-3  | 0            |
| COS       | -7.19521E-3  | -8.66294E-5   | -1.43904E-3  | 0           | -1.91896E-3  |
| CS2       | .06525       | 6.20266E-4    | 1.03038E-2   | 0           | 0            |
| SO2       | 9.63511E-3   | 1.08755E-4    | 0            | 0           | 4.81755E-3   |
| Water     | .87688       | 2.43635E-2    | 0            | .09742      | .77946       |
| Other     | 0            | 99.3315       | 0            | 0           | 0            |
| Gas Total:| 31.0161      | 100           | 24.7039      | 3.13720     | 2.88267      |

# TABLE A-44

PYROLYSIS SUMMARY REPORT    -    USARUN 184

RUN CONDITIONS
---------------
2985 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 100.194 liters

## JP8X-2429 (30% aromatic)
## Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
------------------------------

|         | Dry Wt. % |
|---------|-----------|
| Char    | .51926    |
| Tar     | 13.2663   |
| Gas     | 61.7169   |
| Water   | 3.94470   |
| Missing | 20.5527   |

GAS COMPOSITION
----------------

|            | Dry Wt. % | Volume % | %C | %H | %O |
|------------|-----------|----------|------|---------|---------|
| Methane    | 8.32198   | .38574   | 6.24148 | 2.08049 | 0 |
| CO         | 1.45834   | 3.86277E-2 | .62504 | 0 | .83329 |
| Hydrogen   | 1.38693   | .49537   | 0 | 1.38693 | 0 |
| CO2        | 0         | 0        | 0 | 0 | 0 |
| Acetylene  | 5.25963   | .14504   | 4.85516 | .40446 | 0 |
| Ethylene   | 17.6326   | .46697   | 15.1129 | 2.51970 | 0 |
| Ethane     | 1.23543   | 3.05419E-2 | .98834 | .24708 | 0 |
| Propylene  | 4.92462   | .06340   | 4.22089 | .70372 | 0 |
| Benzene    | 14.6672   | .13946   | 13.5393 | 1.12791 | 0 |
| Paraffins  | .60301    | 9.64332E-3 | .51604 | .08617 | 0 |
| Olefins    | 6.23115   | .08890   | 5.34072 | .89043 | 0 |
| HCN        | 0         | 0        | 0 | 0 | 0 |
| Ammonia    | 0         | 0        | 0 | 0 | 0 |
| COS        | 0         | 0        | 0 | 0 | 0 |
| CS2        | 0         | 0        | 0 | 0 | 0 |
| SO2        | 0         | 0        | 0 | 0 | 0 |
| Water      | 3.94470   | .11252   | 0 | .43825 | 3.50644 |
| Other      | 0         | 98.1467  | 0 | 0 | 0 |
| Gas Total: | 65.6616   | 100      | 51.4407 | 9.88518 | 4.33974 |

# TABLE A-45

| RUN CONDITIONS | Gas Scans => 0 - 0 - 76    0 : 0 |
|---|---|
| --------------- | Analysis => 6 - 30 - 87    0 : 20 |
|  | Stored => 7 - 7 - 87    17 : 49 |

3200 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
758 mm. Final Pressure for 97.3030 liters

## JP8X-2429 (30% aromatic)
## Injector 46 cm Above Extractor

PIROLYSIS PRODUCT DISTRIBUTION
---------------------------------

| | Dry Wt. % |
|---|---|
| | --------- |
| Char | 17.6562 |
| Tar | 6 |
| Gas | 71.8223 |
| Water | 1.89638 |
| Missing | 2.62500 |

GAS COMPOSITION
---------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| | --------- | -------- | | | |
| Methane | 9.18750 | .45250 | 6.89062 | 2.29687 | 0 |
| CO | 4.18258 | .12213 | 1.79265 | 0 | 2.38993 |
| Hydrogen | 3.90625 | 1.54089 | 0 | 3.90625 | 0 |
| CO2 | .28125 | 5.01319E-3 | .07669 | 0 | .20455 |
| Acetylene | 9.81250 | .29815 | 9.05791 | .75458 | 0 |
| Ethylene | 10.7320 | .31337 | 9.19839 | 1.53360 | 0 |
| Ethane | .27133 | 7.39479E-3 | .21706 | 5.42664E-2 | 0 |
| Propylene | .98457 | 1.91667E-2 | .84388 | .14069 | 0 |
| Benzene | 12.2995 | .12892 | 11.3537 | .94583 | 0 |
| Paraffins | 1.67103 | 1.62649E-2 | 1.43224 | .23879 | 0 |
| Olefins | 18.4684 | .17976 | 15.8293 | 2.63914 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 1.89638 | 5.96348E-2 | 0 | .21060 | 1.68570 |
| Other | 0 | 98.3487 | 0 | 0 | 0 |
| | --------- | --------- | | | |
| Gas Total: | 73.7187 | 100 | 56.6925 | 12.7207 | 4.28018 |

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# TABLE A-46

Gas Scans =>  0 - 0 - 76      0 : 0
Analysis =>  6 - 11 - 87     14 : 21
Stored =>  6 - 12 - 87     10 : 26

**RUN CONDITIONS**
------------------

2890 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
759 mm. Final Pressure for 94.4130 liters

## JP8X-2429 (30% aromatic)
## Injector 56 cm Above Extractor

**PYROLYSIS PRODUCT DISTRIBUTION**
---------------------------------

| | Dry Wt. % |
|---|---|
| Char | 36.1937 |
| Tar | 4.18685 |
| Gas | 48.4437 |
| Water | 2.83652 |
| Missing | 8.33910 |

**GAS COMPOSITION**
-------------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 6.33218 | .28998 | 4.74913 | 1.58304 | 0 |
| CO | 4.13964 | .11124 | 1.77425 | 0 | 2.36539 |
| Hydrogen | 7.47404 | 2.74835 | 0 | 7.47404 | 0 |
| CO2 | .23875 | 3.95256E-3 | .06510 | 0 | .17364 |
| Acetylene | 9.65397 | .27299 | 8.91158 | .74239 | 0 |
| Ethylene | 2.19376 | 5.89538E-2 | 1.88027 | .31348 | 0 |
| Ethane | 2.36372E-3 | 5.92865E-5 | 1.89098E-3 | 4.72745E-4 | 0 |
| Propylene | .34886 | 6.25011E-3 | .29901 | 4.98527E-2 | 0 |
| Benzene | 14.6533 | .14135 | 13.5264 | 1.12684 | 0 |
| Paraffins | .26124 | 2.34015E-3 | .22391 | 3.73315E-2 | 0 |
| Olefins | 3.15995 | 2.83062E-2 | 2.70839 | .45155 | 0 |
| HCN | 0 | 0 | 0 | 0 | 0 |
| Ammonia | 0 | 0 | 0 | 0 | 0 |
| COS | 0 | 0 | 0 | 0 | 0 |
| CS2 | 0 | 0 | 0 | 0 | 0 |
| SO2 | 0 | 0 | 0 | 0 | 0 |
| Water | 2.83652 | .08209 | 0 | .31513 | 2.52139 |
| Other | 0 | 99.1876 | 0 | 0 | 0 |
| Gas Total: | 51.2802 | 100 | 34.1400 | 12.0941 | 5.06043 |

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# TABLE A-47

RUN CONDITIONS
-----------------

2610 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1500 Degrees C. @ 0 torr with ALTUBE grid
764 mm. Final Pressure for 100.194 liters

Gas Scans = 0 - 0 - 76    0 : 0
Analysis = 0 - 0 - 76    0 : 0
Stored => 11 - 23 - 87    8 : 56

## JP8X-2429 (30% aromatic)
## Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-----------------------------

|          | Dry Wt. % |
|----------|-----------|
| Char     | 38.4674   |
| Tar      | 5.17241   |
| Gas      | 38.1797   |
| Water    | .82406    |
| Missing  | 17.3563   |

GAS COMPOSITION
----------------

| | Dry Wt. % | | Volume % | %C | %H | %O |
|---|---|---|---|---|---|---|
| Methane   | 4.11411     | | .15412      | 3.49558      | 1.02952       | 0        |
| CO        | 3.95801     | | .98226      | 2.65011      | 0             | 2.14989  |
| Hydrogen  | 7.55233     | | 2.38053     | 0            | 2.65283       | 0        |
| N2        | .19252      | | 5.01047E-3  | 5.22413E-2   | 0             | .15932   |
| Acetylene | 9.38348     | | .21535      | 9.20533      | .68355        | 0        |
| Ethylene  | .71787      | | 1.03098E-2  | .61694       | .13386        | 0        |
| Ethane    | 3.24659E-4  | | 6.92679E-6  | 2.56094E-4   | 5.41736E-5    | 0        |
| Propylene | .34595      | | 1.45827E-3  | .68224       | 1.37133E-2    | 0        |
| Benzene   | 11.9923     | | .89594      | 11.0701      | .92221        | 0        |
| Paraffins | .22446      | | 1.70257E-3  | .19284       | 5.20188E-2    | 0        |
| Olefins   | .71662      | | 5.44532E-3  | .61421       | .10240        | 0        |
| HCN       | 0           | | 0           | 0            | 0             | 0        |
| Ammonia   | 0           | | 0           | 0            | 0             | 0        |
| COS       | 0           | | 0           | 0            | 0             | 0        |
| CS2       | 0           | | 0           | 0            | 0             | 0        |
| SO2       | 0           | | 0           | 0            | 0             | 0        |
| Water     | .82406      | | 2.02302E-2  | 0            | 0             | 0        |
| Other     | 0           | | 99.2085     | 0            | .09155        | .73251   |
| Gas Total: | 39.0038    | | 100         | 25.5691      | 10.6397       | 3.02174  |

## TABLE A-48

RUN CONDITIONS
---------------

Gas Scans =)  0 - 0 - 76    0 : 0
Analysis =>  9 - 23 - 85    12 : 45
Stored =>  9 - 24 - 85    11 : 1

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1100 Degrees c. @ 0 torr with ALTUBE grid
763 mm. Final Pressure for 107.901 liters

### Butane 1100°C
### Injector 6 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
--------------------------------

|  | Dry Wt. % |
|---|---|
| Char | 0 |
| Tar | .16271 |
| Gas | 99.2707 |
| Water | 2.15419E-2 |
| Missing | .54502 |

GAS COMPOSITION
-----------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | .08235 | 7.33469E-3 | 6.17687E-2 | 2.05895E-2 | 0 |
| CO | 3.93079E-2 | 2.00040E-3 | 1.68473E-2 | 0 | 2.24605E-2 |
| Hydrogen | 0 | 0 | 0 | 0 | 0 |
| CO2 | .21994 | 7.12284E-3 | 5.99786E-2 | 0 | .15996 |
| Acetylene | 2.36473E-2 | 1.29599E-3 | 2.18288E-2 | 1.81847E-3 | 0 |
| Ethylene | .31911 | 1.50065E-2 | .27351 | 4.53015E-2 | 0 |
| Ethane | .06793 | 3.00131E-3 | 5.43443E-2 | 1.35860E-2 | 0 |
| Propylene | .27832 | 9.44278E-3 | .23855 | 3.97728E-2 | 0 |
| Benzene | 3.01218E-2 | 5.50277E-4 | 2.78054E-2 | 2.31637E-3 | 0 |
| Paraffins | 98.0789 | 2.21300 | 84.0635 | 14.0154 | 0 |
| Olefins | .12480 | 3.49934E-3 | .10696 | 1.78342E-2 | 0 |
| HCN | 1.20522E-2 | 6.36064E-4 | 5.35604E-3 | 4.45935E-4 | 0 |
| Ammonia | -8.80703E-4 | -7.38202E-5 | 0 | -1.55444E-4 | 0 |
| COS | -1.33358E-3 | -3.16711E-5 | -2.66716E-4 | 0 | -3.55666E-4 |
| CS2 | -.08665 | -1.62468E-3 | -1.36826E-2 | 0 | 0 |
| SO2 | .18697 | 4.16302E-3 | 0 | 0 | .09348 |
| Water | 2.15419E-2 | 1.18061E-3 | 0 | 2.39331E-3 | 1.91486E-2 |
| Other | 0 | 97.6963 | 0 | 0 | 0 |
| Gas Total: | 99.2922 | 100 | 84.9165 | 14.1596 | .29470 |

PYROLYSIS SUMMARY REPORT   -   USARUN 50

RUN CONDITIONS
----------------

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1100 Degrees c. @ 0 torr with ALTUBE grid
762 mm. Final Pressure for 107.901 liters

Gas Scans => 0 - 0 - 76     0 : 0
Analysis => 9 - 23 - 85    10 : 16
Stored => 9 - 24 - 85    11 : 0

## Butane 1100°C
## Injector 16 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-------------------------------

| | Dry Wt. % |
|---|---|
| Char | 0 |
| Tar | .23222 |
| Gas | 92.9904 |
| Water | 5.22053E-2 |
| Missing | 6.72511 |

GAS COMPOSITION
----------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 1.28010 | .11415 | .96007 | .32002 | 0 |
| CO | .31180 | 1.58885E-2 | .13363 | 0 | .17816 |
| Hydrogen | .43601 | .28699 | 0 | .43601 | 0 |
| CO2 | .13443 | 4.35949E-3 | 3.66614E-2 | 0 | .09777 |
| Acetylene | .10950 | 6.00951E-3 | .10108 | 8.42121E-3 | 0 |
| Ethylene | 4.19399 | .21371 | 3.59457 | .59932 | 0 |
| Ethane | .63981 | 2.80052E-2 | .51184 | .12796 | 0 |
| Propylene | 2.51816 | .07859 | 2.15832 | .35984 | 0 |
| Benzene | .08169 | 1.49436E-3 | .07541 | 6.28223E-3 | 0 |
| Paraffins | 82.0767 | 1.86994 | 71.0336 | 11.8430 | 0 |
| Olefins | .40758 | 1.43963E-2 | .34933 | 5.82436E-2 | 0 |
| HCN | 2.22047E-2 | 1.17339E-3 | 9.86777E-3 | 8.21574E-4 | 0 |
| Ammonia | 1.82423E-3 | 1.53107E-4 | 0 | 3.21978E-4 | 0 |
| COS | -1.12255E-3 | -2.66943E-5 | -2.24519E-4 | 0 | -2.99384E-4 |
| CS2 | -.07560 | -1.41947E-3 | -1.19387E-2 | 0 | 0 |
| SO2 | .16075 | 3.58373E-3 | 0 | 0 | .08037 |
| Water | 5.22053E-2 | 2.86487E-3 | 0 | 5.80001E-3 | 4.64053E-2 |
| Other | 0 | 96.8484 | 0 | 0 | 0 |
| Gas Total: | 93.0426 | 100 | 78.9524 | 13.7661 | .40242 |

# TABLE A-50

**RUN CONDITIONS**

|  |
|---|
| Gas Scans => 0 - 0 - 76    0 : 0 |
| Analysis => 9 - 23 - 85    15 : 1 |
| Stored => 9 - 24 - 85    11 : 3 |

----------------

6330 mg. NO COAL
0 sec. 0 0 Amps
0 sec. 0 0 Amps
1100 Degrees c. 0 0 torr with ALTUBE grid
763 mm. Final Pressure for 109.828 liters

## Butane 1100°C
## Injector 26 cm Above Extractor

**PYROLYSIS PRODUCT DISTRIBUTION**

--------------------------------

|  | Dry Wt. % |
|---|---|
| Char | 0 |
| Tar | .11532 |
| Gas | 97.8934 |
| Water | .58208 |
| Missing | 1.40916 |

**GAS COMPOSITION**

----------------

|  | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 6.80943 | .59780 | 5.10707 | 1.70235 | 0 |
| CO | .86749 | 4.35185E-2 | .37180 | 0 | .49568 |
| Hydrogen | 1.19431 | .77300 | 0 | 1.19431 | 0 |
| CO2 | 6.20118E-4 | 1.97965E-5 | 1.69106E-4 | 0 | 4.51012E-4 |
| Acetylene | .78706 | 4.25209E-2 | .72653 | 6.05251E-2 | 0 |
| Ethylene | 22.3175 | 1.02900 | 19.1283 | 3.18917 | 0 |
| Ethane | 2.11532 | .09099 | 1.69225 | .42306 | 0 |
| Propylene | 8.63033 | .26460 | 7.39705 | 1.23327 | 0 |
| Benzene | 1.39716 | 2.51604E-2 | 1.28972 | .10744 | 0 |
| Paraffins | 51.7867 | 1.14799 | 44.3864 | 7.40032 | 0 |
| Olefins | 1.98894 | 5.46002E-2 | 1.70472 | .28421 | 0 |
| HCN | -5.46550E-2 | -2.84337E-3 | -2.42887E-2 | -2.02223E-3 | 0 |
| Ammonia | 1.44423E-2 | 1.19332E-3 | 0 | 2.54908E-3 | 0 |
| COS | -3.77467E-4 | -8.83680E-6 | -7.54934E-5 | 0 | -1.00670E-4 |
| CS2 | -4.81884E-2 | -8.90628E-4 | -7.60896E-3 | 0 | 0 |
| SO2 | 4.50622E-2 | 9.89007E-4 | 0 | 0 | 2.25311E-2 |
| Water | .58208 | 3.14472E-2 | 0 | .06467 | .51741 |
| Other | 0 | 95.0854 | 0 | 0 | 0 |
| Gas Total: | 98.4755 | 100 | 81.7721 | 15.6598 | 1.03598 |

# TABLE A-51

Gas Scans =>  0 - 0 - 76     0 : 0
Analysis =>  9 - 19 - 85    15 : 50
Stored =>  9 - 24 - 85    11 : 3

RUN CONDITIONS
------------------

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1100 Degrees c. @ 0 torr with ALTUBE grid
764 mm. Final Pressure for 111.754 liters


## Butane 1100°C
## Injector 36 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-------------------------------

|            | Dry Wt. %   |
|------------|-------------|
| Char       | 0           |
| Tar        | 1.11058     |
| Gas        | 100.159     |
| Water      | .53258      |
| Missing    | -1.80252    |

GAS COMPOSITION
-----------------

|           | Dry Wt. %    | Volume %      | %C          | %H          | %O          |
|-----------|--------------|---------------|-------------|-------------|-------------|
| Methane   | 13.1714      | 1.14633       | 9.87861     | 3.29287     | 0           |
| CO        | 1.13014      | 5.62050E-2    | .48438      | 0           | .64576      |
| Hydrogen  | 1.73775      | 1.10599       | 0           | 1.73775     | 0           |
| CO2       | 8.54349E-4   | 2.70384E-5    | 2.32980E-4  | 0           | 6.21368E-4  |
| Acetylene | 3.05213      | .14900        | 2.81742     | .23470      | 0           |
| Ethylene  | 39.3254      | 1.78193       | 33.7058     | 5.61960     | 0           |
| Ethane    | 1.96011      | .09098        | 1.56809     | .39202      | 0           |
| Propylene | 9.29383      | .27999        | 7.96574     | 1.32808     | 0           |
| Benzene   | 7.26917      | .12977        | 6.71017     | .55899      | 0           |
| Paraffins | 20           | .43573        | 17.1420     | 2.85800     | 0           |
| Olefins   | 3.21800      | .08680        | 2.75815     | .45985      | 0           |
| HCN       | -1.17424E-2  | -6.05608E-4   | -5.21833E-3 | -4.34469E-4 | 0           |
| Ammonia   | 3.03197E-2   | 2.48355E-3    | 0           | 5.35142E-3  | 0           |
| COS       | 2.91963E-3   | 6.77602E-5    | 5.83926E-4  | 0           | 7.78665E-4  |
| CS2       | -3.02831E-2  | -5.54863E-4   | -4.78171E-3 | 0           | 0           |
| SO2       | -.06460      | -1.40574E-3   | 0           | 0           | -3.23041E-2 |
| Water     | .53258       | 2.85241E-2    | 0           | 5.91699E-2  | .47341      |
| Other     | 0            | 96.1126       | 0           | 0           | 0           |
| Gas Total:| 100.691      | 100           | 83.0212     | 16.5459     | 1.08827     |

A-53

PYROLYSIS SUMMARY REPORT  -  USARUN 49

RUN CONDITIONS
-----------------

Gas Scans =>  0 - 0 - 76     0 : 0
Analysis =>  9 - 20 - 85    11 : 17
Stored =>  9 - 24 - 85    11 : 6

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1100 Degrees c. @ 0 torr with ALTUBE grid
763.500 mm. Final Pressure for 111.754 liters

## Butane 1100°C
## Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
-------------------------------

|        | Dry Wt. % |
|--------|-----------|
| Char   | 0         |
| Tar    | 1.34439   |
| Gas    | 99.4801   |
| Water  | .62093    |
| Missing| -1.44549  |

GAS COMPOSITION
---------------

| | Dry Wt. % | Volume % | %C | %H | %O |
|---|---|---|---|---|---|
| Methane | 16.1035 | 1.38846 | 12.0776 | 4.02588 | 0 |
| CO | 1.17077 | 5.76830E-2 | .58179 | 0 | .66898 |
| Hydrogen | 2.18325 | 1.38899 | 0 | 2.18325 | 0 |
| CO2 | 5.09491E-4 | 1.59741E-5 | 1.38938E-4 | 0 | 3.70552E-4 |
| Acetylene | 4.87361 | .23799 | 4.49883 | .37478 | 0 |
| Ethylene | 45.4391 | 2.05907 | 38.9459 | 6.49325 | 0 |
| Ethane | 1.93945 | .08918 | 1.55156 | .38789 | 0 |
| Propylene | 7.13586 | .21499 | 6.11614 | 1.01971 | 0 |
| Benzene | 9.18586 | .16246 | 8.47947 | .70639 | 0 |
| Paraffins | 8.32701 | .18140 | 7.13708 | 1.18993 | 0 |
| Olefins | 3.12164 | .08420 | 2.67556 | .44608 | 0 |
| HCN | 4.80294E-2 | 2.45401E-3 | 2.13443E-2 | 1.77709E-3 | 0 |
| Ammonia | 3.04464E-2 | 2.47070E-3 | 0 | 5.37380E-3 | 0 |
| COS | 3.20588E-3 | 7.37104E-5 | 6.41176E-4 | 0 | 8.55009E-4 |
| CS2 | 2.05354E-3 | 3.72753E-5 | 3.24254E-4 | 0 | 0 |
| SO2 | -.09417 | -2.02986E-3 | 0 | 0 | -4.70853E-2 |
| Water | .62093 | 3.29463E-2 | 0 | .06898 | .55195 |
| Other | 0 | 96.0696 | 0 | 0 | 0 |
| Gas Total: | 100.101 | 100 | 82.0064 | 16.9033 | 1.17507 |

PYROLYSIS SUMMARY REPORT  -  USARUN 53

RUN CONDITIONS
----------------

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1100 Degrees C. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 111.754 liters

Gas Scans =) 0 - 0 - 76    0 : 0
Analysis =) 9 - 24 - 85    12 : 24
Stored =) 9 - 24 - 85    14 : 11

Butane 1100°C
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION
--------------------------------

|  | Dry Wt. % |
| --- | --- |
| Char | 0 |
| Tar | 2.06161 |
| Gas | 101.160 |
| Water | .40364 |
| Missing | -3.62559 |

GAS COMPOSITION
----------------

| | Dry Wt. % | Volume % | %C | %H | %O |
| --- | --- | --- | --- | --- | --- |
| Methane | 18.8035 | 1.63517 | 14.1026 | 4.70087 | 0 |
| CO | 1.92398 | .09560 | .82461 | 0 | 1.09936 |
| Hydrogen | 2.96998 | 1.88996 | 0 | 2.96998 | 0 |
| CO2 | 1.52052E-4 | 4.80824E-6 | 4.14646E-5 | 0 | 1.10587E-4 |
| Acetylene | 6.90205 | .33700 | 6.37128 | .53076 | 0 |
| Ethylene | 46.2985 | 2.09801 | 39.6825 | 6.61606 | 0 |
| Ethane | 1.75072 | .08119 | 1.40057 | .35014 | 0 |
| Propylene | 5.11848 | .15420 | 4.38705 | .73143 | 0 |
| Benzene | 10.7317 | .19143 | 9.90647 | .82527 | 0 |
| Paraffins | 3.69036 | .08039 | 3.16301 | .52735 | 0 |
| Olefins | 2.97788 | .08030 | 2.55234 | .42553 | 0 |
| HCN | .23271 | 1.19925E-2 | .10342 | 8.61058E-3 | 0 |
| Ammonia | 3.19180E-2 | 2.61235E-3 | 0 | 5.63353E-3 | 0 |
| COS | 2.54749E-3 | 5.90755E-5 | 5.09498E-4 | 0 | 6.79416E-4 |
| CS2 | -2.61289E-3 | -4.78359E-5 | -4.12576E-4 | 0 | |
| SO2 | -.10271 | -2.23306E-3 | 0 | 0 | -5.13576E-2 |
| Water | .40364 | 2.16010E-2 | 0 | 4.48452E-2 | .35880 |
| Other | 0 | 95.7627 | 0 | 0 | 0 |
| Gas Total: | 101.563 | 100 | 82.4940 | 17.7365 | 1.40759 |

# TABLE A-54

RUN CONDITIONS
---------------

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1100 Degrees c. @ 0 torr with ALTUBE grid
764 mm. Final Pressure for 111.754 liters

Gas Scans =>  0 - 0 - 76    0 : 0
Analysis =>  9 - 19 - 85    10 : 59
Stored =>  9 - 24 - 85    11 : 7

**Butane 1100°C**
**Injector 66 cm Above Extractor**

PYROLYSIS PRODUCT DISTRIBUTION
--------------------------------

|          | Dry Wt. % |
|----------|-----------|
| Char     | 5.52922E-2 |
| Tar      | 3.95892   |
| Gas      | 97.1055   |
| Water    | .52797    |
| Missing  | -1.64770  |

GAS COMPOSITION
---------------

|           | Dry Wt. % | Volume % | %C | %H | %O |
|-----------|-----------|----------|------|------|------|
| Methane   | 17.3260   | 1.49289 | 12.9945 | 4.33151 | 0 |
| CO        | 1.52801   | .07523 | .65490 | 0 | .87310 |
| Hydrogen  | 3.60821   | 2.29581 | 0 | 3.60821 | 0 |
| CO2       | 1.71049E-4 | 5.35942E-6 | 4.66452E-5 | 0 | 1.24404E-4 |
| Acetylene | 9.87045   | .48206 | 9.11142 | .75903 | 0 |
| Ethylene  | 44.1374   | 2 | 37.8302 | 6.30724 | 0 |
| Ethane    | 1.23605   | 5.68020E-2 | .98884 | .24721 | 0 |
| Propylene | 5.53063   | .18154 | 4.74030 | .79032 | 0 |
| Benzene   | 11.1255   | .19664 | 10.2699 | .85555 | 0 |
| Paraffins | .38072    | 8.29842E-3 | .32632 | 5.44058E-2 | 0 |
| Olefins   | 2.36176   | .06370 | 2.02427 | .33749 | 0 |
| HCN       | .49473    | 2.52613E-2 | .21985 | 1.83051E-2 | 0 |
| Ammonia   | 3.07899E-2 | 2.49686E-3 | 0 | 5.43427E-3 | 0 |
| COS       | 2.66313E-3 | 6.11914E-5 | 5.32627E-4 | 0 | 7.10258E-4 |
| CS2       | 1.02401E-2 | 1.85755E-4 | 1.61691E-3 | 0 | 0 |
| SO2       | -.09832   | -2.11796E-3 | 0 | 0 | -4.91610E-2 |
| Water     | .52797    | 2.79953E-2 | 0 | 5.86576E-2 | .46931 |
| Other     | 0         | 96.0398 | 0 | 0 | 0 |
| Gas Total: | 97.6334  | 100 | 79.1628 | 17.3734 | 1.29409 |

```
                                                Gas Scans =>  0 - 0 - 76      0 : 0
RUN CONDITIONS                                  Analysis =>  10 - 22 - 85    10 : 9
---------------                                 Stored =>   10 - 22 - 85    12 : 46
  6330 mg. ASIS COAL
  0 sec. @ 0 Amps
  0 sec. @ 0 Amps
  1300 Degrees c. @ 0 torr with ALTUBE grid
  764 mm. Final Pressure for 96.3400 liters
```

Butane 1300°C
Injector 6 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	0
Tar	.12954
Gas	96.3407
Water	5.73878E-2
Missing	3.47235

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	1.16814	.11558	.87610	.29203	0
CO	.58871	3.32858E-2	.25232	0	.33639
Hydrogen	.36571	.27000	0	.36571	0
CO2	7.69844E-3	2.76987E-4	2.09936E-3	0	5.59907E-3
Acetylene	.23394	1.42446E-2	.21595	1.79904E-2	0
Ethylene	4.26744	.24127	3.65763	.60981	0
Ethane	.71516	3.70000E-2	.57213	.14303	0
Propylene	2.06919	.07904	1.77350	.29568	0
Benzene	.17062	3.46305E-3	.15750	1.31210E-2	0
Paraffins	86.0663	2.17500	73.7674	12.2988	0
Olefins	.68396	2.13999E-2	.58622	.09773	0
HCN	3.35735E-2	1.96853E-3	1.49200E-2	1.24222E-3	0
Ammonia	4.23767E-3	3.94628E-4	0	7.47948E-4	0
COS	-1.92490E-3	-5.07888E-5	-3.84981E-4	0	-5.13372E-4
CS2	-5.57909E-2	-1.16214E-3	-8.80939E-3	0	0
SO2	.14230	3.52017E-3	0	0	.07115
Water	5.73878E-2	3.49427E-3	0	6.37578E-3	5.10120E-2
Other	0	99.2194	0	0	0
Gas Total:	96.3981	100	81.8666	14.1423	.46364

PYROLISIS SUMMARY REPORT - USARUN 60

RUN CONDITIONS

Gas Scans =) 0 - 0 - 76   0 : 0
Analysis =) 10 - 21 - 85   15 : 15
Stored =) 10 - 21 - 85   16 : 30

6330 mg. ASIS COAL
0 sec. 0 0 Amps
0 sec. 0 0 Amps
1300 Degrees c. 0 0 torr with ALTUBE grid
767 mm. Final Pressure for 98.2668 liters

Butane 1300°C
Injector 16 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	0
Tar	.71090
Gas	103.520
Water	.46810
Missing	-4.69984

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	7.34356	.71919	5.50767	1.83589	0
CO	2.17730	.12104	.93319	0	1.24411
Hydrogen	1.24170	.89895	0	1.24170	0
CO2	1.62526E-4	5.78802E-6	4.43211E-5	0	1.18205E-4
Acetylene	1.90168	.11460	1.75544	.14623	0
Ethylene	22.3522	1.24993	19.1581	3.19414	0
Ethane	1.17206	6.12192E-2	.93765	.23441	0
Propylene	7.95892	.29804	6.82159	1.13733	0
Benzene	1.86229	3.74119E-2	1.71908	.14321	0
Paraffins	55.2717	1.36940	47.3733	7.89832	0
Olefins	2.24012	.06869	1.92001	.32011	0
HCN	1.52312E-2	8.83950E-4	6.76874E-3	5.63554E-4	0
Ammonia	1.80596E-2	1.66463E-3	0	3.18752E-3	0
COS	-1.31309E-4	-3.42928E-6	-2.62619E-5	0	-3.50203E-5
CS2	-.07036	-1.45084E-3	-1.11111E-2	0	0
SO2	4.24677E-2	1.03974E-3	0	0	2.12338E-2
Water	.46810	2.82116E-2	0	5.20066E-2	.41609
Other	0	94.9223	0	0	0
Gas Total:	103.988	100	86.1218	16.2071	1.68152

PYROLYSIS SUMMARY REPORT   -   USARUN 59

RUN CONDITIONS

```
Gas Scans =>  0 - 0 - 76     0 : 0
Analysis =>  10 - 21 - 85    13 : 35
Stored  =>  10 - 21 - 85     16 : 12
```

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
767 mm. Final Pressure for 100.193 liters

Butane 1300°C
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	.36492
Tar	.60821
Gas	99.7940
Water	.33238
Missing	-1.09952

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	14.2606	1.26899	10.6954	3.56516	0
CO	2.99750	.16342	1.28473	0	1.71277
Hydrogen	2.26224	1.60599	0	2.26224	0
CO2	3.28682E-4	1.14033E-5	8.96316E-5	0	2.39050E-4
Acetylene	4.68404	.26897	4.32384	.36020	0
Ethylene	40.1374	2.18604	34.4018	5.73564	0
Ethane	1.97448	.10047	1.57959	.39489	0
Propylene	8.11532	.29809	6.95564	1.15967	0
Benzene	6.52868	.12777	6.02662	.50205	0
Paraffins	15.2069	.36950	13.0338	2.17307	0
Olefins	3.62717	.10910	3.10884	.51832	0
HCN	.13037	7.37140E-3	5.79400E-2	4.82398E-3	0
Ammonia	2.93450E-2	2.63508E-3	0	5.17939E-3	0
COS	2.62408E-3	6.67629E-5	5.24816E-4	0	6.99842E-4
CS2	-2.44300E-2	-4.90703E-4	-3.85749E-3	0	0
SO2	-.07779	-1.85556E-3	0	0	-3.88971E-2
Water	.33238	1.95154E-2	0	3.69280E-2	.29545
Other	0	95.2976	0	0	0
Gas Total:	100.126	100	81.4651	16.7102	1.97027

TABLE A-58

RUN CONDITIONS

Gas Scans =) 0 - 0 - 76   0 : 0
Analysis =) 10 - 8 - 85   0 : 43
Stored =) 10 - 8 - 85   12 : 30

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
773.700 mm. Final Pressure for 100.194 liters

COAL

Butane 1300°C
Injector 36 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	3.40916
Tar	1.50078
Gas	88.9245
Water	.25395
Missing	5.91153

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	17.4945	1.63796	13.1209	4.37363	0
CO	3.56384	.19067	1.52746	0	2.03638
Hydrogen	4.30173	3.05286	0	4.30173	0
CO2	.23652	8.05277E-3	.06450	0	.17202
Acetylene	10.6903	.61399	9.86827	.82208	0
Ethylene	34.7030	1.89000	29.7439	4.95905	0
Ethane	.98578	4.89983E-2	.78862	.19715	0
Propylene	2.13428	.07840	1.82929	.30498	0
Benzene	10.6673	.20487	9.84704	.82031	0
Paraffins	.95892	2.32906E-2	.82189	.13703	0
Olefins	3.39652	.10219	2.91116	.48536	0
HCN	.70767	3.92638E-2	.31449	2.61840E-2	0
Ammonia	2.73433E-2	2.40948E-3	0	4.82609E-3	0
COS	1.05602E-3	2.63660E-5	2.11205E-4	0	2.81642E-4
CS2	4.08370E-3	8.04936E-5	6.44816E-4	0	0
SO2	-.08149	-1.90760E-3	0	0	-4.07489E-2
Water	.25395	1.46321E-2	0	2.82145E-2	.22574
Other	0	89.8510	0	0	0
Gas Total:	89.1705	100	70.8384	16.4606	2.39368

TABLE A-59

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 10 - 20 - 85   12 : 45
Stored => 10 - 20 - 85   14 : 14

RUN CONDITIONS

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
768.700 mm. Final Pressure for 98.2670 liters

Butane 1300°C
Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	6.93680
Tar	2.16429
Gas	84.7075
Water	.22133
Missing	5.96998

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	17.0233	1.64123	12.7674	4.25582	0
CO	3.54817	.19547	1.52074	0	2.02742
Hydrogen	5.54502	4.01300	0	5.54502	0
CO2	.94773	3.32260E-2	.25844	0	.68928
Acetylene	15.7109	.91999	14.5027	1.20816	0
Ethylene	29.1548	1.61896	24.9885	4.16622	0
Ethane	.45593	2.34438E-2	.36474	.09118	0
Propylene	.35545	1.32951E-2	.30465	5.07938E-2	0
Benzene	10.8325	.21423	9.99950	.83302	0
Paraffins	0	0	0	0	0
Olefins	1.35545	4.16027E-2	1.16175	.19369	0
HCN	1.04893	5.99278E-2	.46614	3.88104E-2	0
Ammonia	2.16443E-2	1.96399E-3	0	3.82021E-3	0
COS	6.60438E-4	1.69795E-5	1.32087E-4	0	1.76138E-4
CS2	-2.19518E-3	-4.45557E-5	-3.46620E-4	0	0
SO2	-5.92128E-2	-1.42718E-3	0	0	-2.96064E-2
Water	.22133	1.31315E-2	0	2.45899E-2	.19674
Other	0	96.2711	0	0	0
Gas Total:	84.9289	100	66.3346	16.4111	2.88402

TABLE A-60

```
                                              Gas Scans =)  0 - 0 - 76    0 : 0
RUN CONDITIONS                                Analysis =)  10 - 21 - 85   10 : 47
---------------                                 Stored =)  10 - 21 - 85   11 : 39

  6330 mg. ASIS COAL
  0 sec. @ 0 Amps
  0 sec. @ 0 Amps
  1300 Degrees c. @ 0 torr with ALTUBE grid
  768 mm. Final Pressure for 98.2668 liters
```

Butane 1300°C
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	9.67140
Tar	1.74565
Gas	77.4432
Water	.70367
Missing	10.4360

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	15.1876	1.45565	11.3907	3.79692	0
CO	3.34437	.18316	1.43339	0	1.91097
Hydrogen	6.34597	4.59244	0	6.34597	0
CO2	.82923	2.89011E-2	.22613	0	.60310
Acetylene	17.2985	1.01302	15.9683	1.33026	0
Ethylene	21.4297	1.18997	18.3673	3.06230	0
Ethane	.17693	8.99739E-3	.14154	3.53870E-2	0
Propylene	1.68878	6.17057E-2	1.44745	.24132	0
Benzene	10.2503	.20152	9.46212	.78825	0
Paraffins	0	0	0	0	0
Olefins	.89257	2.73958E-2	.76502	.12754	0
HCN	1.27366	.07234	.56601	4.71256E-2	0
Ammonia	1.49971E-2	1.35284E-3	0	2.64700E-3	0
COS	-4.84647E-4	-1.23868E-5	-9.69294E-5	0	-1.29255E-4
CS2	1.11203E-2	2.24385E-4	1.75590E-3	0	0
SO2	-3.61862E-2	-8.67065E-4	0	0	-1.80931E-2
Water	.70367	4.15039E-2	0	.07817	.62550
Other	0	95.9905	0	0	0
Gas Total:	78.1469	100	59.7698	15.8559	3.12135

PYROLYSIS SUMMARY REPORT - USARUN 54

	Gas Scans =>	0 - 0 - 76	0 : 0
RUN CONDITIONS	Analysis =>	9 - 24 - 85	20 : 33
	Stored =>	9 - 25 - 85	10 : 31

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
665 mm. Final Pressure for 105.974 liters

Butane 1300°C
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	25.5939
Tar	1.62717
Gas	65.2285
Water	1.06215
Missing	6.48815

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	9.51841	.99363	7.13881	2.37960	0
CO	3.03310	.18093	1.29998	0	1.73311
Hydrogen	11.5924	8.89142	0	11.5924	0
CO2	.70098	2.66098E-2	.19115	0	.50982
Acetylene	21.7693	1.28114	20.0952	1.67406	0
Ethylene	8.26540	.45115	7.08427	1.18112	0
Ethane	1.27013E-5	7.07148E-7	1.01610E-5	2.54026E-6	0
Propylene	0	0	0	0	0
Benzene	10.0899	.21606	9.31406	.77591	0
Paraffins	.11374	2.97744E-3	.09749	1.62540E-2	0
Olefins	.09478	3.08270E-3	.08124	1.35450E-2	0
HCN	1.18561	.07334	.52688	4.38678E-2	0
Ammonia	4.21197E-3	4.13828E-4	0	7.43413E-4	0
COS	-3.15989E-3	-8.79648E-5	-6.31979E-4	0	-8.42744E-4
CS2	2.40891E-3	5.29409E-5	3.80367E-4	0	0
SO2	3.64195E-3	9.50469E-5	0	0	1.82097E-3
Water	1.06215	.06823	0	.11800	.94415
Other	0	97.6647	0	0	0
Gas Total:	66.2906	100	45.8289	17.7955	3.18807

TABLE A-62

RUN CONDITIONS

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1200 Degrees c. @ 0 torr with ALTUBE grid
756 mm. Final Pressure for 104.047 liters

Gas Scans =) 0 - 0 - 76   0 : 0
Analysis =) 10 - 23 - 85   14 : 9
Stored =) 10 - 23 - 85   15 : 20

Butane 1200°C
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	8.33965
Tar	1.53554
Gas	75.2005
Water	.08858
Missing	14.8357

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	15.8525	1.49755	11.8894	3.96313	0
CO	2.63903	.14245	1.13109	0	1.50794
Hydrogen	6.13586	4.19404	0	6.13586	0
CO2	.29039	9.97559E-3	.07919	0	.21120
Acetylene	15.9842	.88399	14.7550	1.22918	0
Ethylene	23.1848	1.21600	19.8717	3.31311	0
Ethane	.23075	1.16260E-2	.18460	4.61509E-2	0
Propylene	4.26540E-2	1.49470E-3	3.65587E-2	6.09526E-3	0
Benzene	9.70413	.18804	8.95788	.74624	0
Paraffins	5.52922E-2	1.29629E-3	4.73909E-2	7.90126E-3	0
Olefins	1.08056	3.12962E-2	.92615	.15441	0
HCN	.99549	5.57285E-2	.44239	3.68332E-2	0
Ammonia	1.77317E-2	1.57654E-3	0	3.12965E-3	0
COS	-1.01306E-3	-2.55203E-5	-2.02612E-4	0	-2.70183E-4
CS2	-2.67721E-3	-5.32442E-5	-4.22732E-4	0	0
SO2	-4.28370E-2	-1.01167E-3	0	0	-2.14185E-2
Water	.08858	5.14986E-3	0	9.84194E-3	.07874
Other	0	88.7920	0	0	0
Gas Total:	75.2891	100	58.3208	15.6519	1.77620

TABLE A-63

```
                                           Gas Scans =)  0 - 0 - 76     0 : 0
RUN CONDITIONS                             Analysis =>  10 - 23 - 85    9 : 46
---------------                            Stored =>   10 - 23 - 85    13 : 10

 6330 mg. ASIS COAL
 0 sec. @ 0 Amps
 0 sec. @ 0 Amps
 1400 Degrees c. @ 0 torr with ALTUBE grid
 759 mm. Final Pressure for 100.193 liters
```

Butane 1400°C
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	44.1879
Tar	.61769
Gas	53.7937
Water	.08463
Missing	1.31595

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	6.68435	.64880	5.01326	1.67108	
CO	3.75836	.20845	1.61083		2.14752
Hydrogen	12.4676	8.84980		12.4676	
CO2	.52475	1.85217E-2	.14310		.38165
Acetylene	19.3507	1.11146	17.8626	1.48806	
Ethylene	2.47600	.13733	2.12218	.35382	
Ethane	1.15549E-4	5.98167E-6	9.24392E-5	2.31098E-5	
Propylene	.18039	6.67031E-3	.15461	2.57780E-2	
Benzene	8.05215	.16032	7.43294	.61921	
Paraffins	.13206	3.21475E-3	.11319	1.88727E-2	
Olefins	.16793	5.04611E-3	.14393	2.39972E-2	
HCN	1.22702	.07057	.54528	4.53999E-2	
Ammonia	2.67612E-3	2.44475E-4		4.72335E-4	
COS	-4.34367E-3	-1.12430E-4	-8.68735E-4		-1.15845E-3
CS2	-1.75352E-2	-3.58323E-4	-2.76881E-3		
SO2	2.16233E-2	5.24711E-4			1.08116E-2
Water	.08463	5.05509E-3		9.40241E-3	.07522
Other	0	98.4553			
	----------	----------			
Gas Total:	53.8783	100	35.1384	16.7237	2.61406
```

PYROLYSIS SUMMARY REPORT — USARUN 55

RUN CONDITIONS

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1500 Degrees c. @ 0 torr with ALTUBE grid
764 mm. Final Pressure for 94.4130 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 9 - 25 - 85   21 : 11
Stored => 15 - 26 - 79   10 : 46

Butane 1500°C
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	50.0742
Tar	1.12164
Gas	46.8425
Water	.22061
Missing	1.74091

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	1.50054	.15355	1.12540	.37513	0
CO	4.90667	.28692	2.10299	0	2.80367
Hydrogen	14.5624	11.9070	0	14.5624	0
CO2	.93751	3.48867E-2	.25566	0	.68185
Acetylene	19.5165	1.12799	18.0157	1.50082	0
Ethylene	2.09790	.12267	1.79811	.29979	0
Ethane	3.75871E-5	2.05686E-6	3.01497E-5	7.53742E-6	0
Propylene	.13258	5.16876E-3	.11364	1.89467E-2	0
Benzene	3.11196	.06532	2.87265	.23930	0
Paraffins	3.15955E-2	7.98429E-4	2.70805E-2	4.51500E-3	0
Olefins	4.42338E-2	1.40052E-3	3.79127E-2	6.32101E-3	0
HCN	1.47117	.08921	.65379	5.44335E-2	0
Ammonia	2.52434E-3	2.43127E-4	0	4.45546E-4	0
COS	-3.09384E-3	-8.44269E-5	-6.18768E-4	0	-8.25127E-4
CS2	2.28469E-2	4.92207E-4	3.60752E-3	0	0
SO2	2.54375E-2	6.50773E-4	0	0	1.27187E-2
Water	.22061	1.38928E-2	0	2.45101E-2	.19610
Other	0	90.7502	0	0	0
Gas Total:	47.0631	100	27.0060	17.0866	3.69352

TABLE A-65

RUN CONDITIONS

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 11 - 22 - 85   9 : 8
Stored => 11 - 22 - 85   9 : 52

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
763 mm. Final Pressure for 100.193 liters

Butane 1300°C with H2
Injector 6 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	0
Tar	.18957
Gas	101.091
Water	1.02586
Missing	-2.30647

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	1.27951	.12189	.95963	.31987	0
CO	.41775	2.27410E-2	.17905	0	.23870
Hydrogen	3.50858	2.49095	0	3.50868	0
CO2	3.18397E-4	1.10296E-5	8.68268E-5	0	2.31570E-4
Acetylene	.22380	1.31203E-2	.20659	1.72107E-2	0
Ethylene	3.37914	.18359	2.89626	.48288	0
Ethane	.34123	1.69986E-2	.27294	.06824	0
Propylene	1.57030	5.27064E-2	1.34590	.22439	0
Benzene	.11898	2.32513E-3	.10983	9.15004E-3	0
Paraffins	90.5782	2.20104	77.6345	12.9436	0
Olefins	.26540	7.99475E-3	.22747	3.79260E-2	0
HCN	8.97843E-3	5.06853E-4	3.99001E-3	3.32202E-4	0
Ammonia	5.60756E-3	5.02772E-4	0	9.89735E-4	0
COS	-1.21007E-3	-3.07401E-5	-2.42014E-4	0	-3.22726E-4
CS2	-5.77889E-2	-1.15898E-3	-9.12488E-3	0	0
SO2	.15698	3.73871E-3	0	0	.07849
Water	1.02586	6.01397E-2	0	.11397	.91188
Other	0	98.9648	0	0	0
Gas Total:	102.116	100	83.8270	17.7272	1.22899

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TABLE A-66

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 11 - 22 - 85   7 : 17
Stored => 11 - 22 - 85   8 : 8

RUN CONDITIONS

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
766 mm. Final Pressure for 100.193 liters

Butane 1300°C with H2
Injector 16 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	0
Tar	.33965
Gas	95.6849
Water	.37039
Missing	3.60505

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	8.99687	.85082	6.74765	2.24921	0
CO	1.13171	6.11567E-2	.48505	0	.64666
Hydrogen	4.58072	3.10966	0	3.58072	0
CO2	4.738E-4	1.63302E-5	1.29497E-4	0	3.45375E-4
Acetylene	1.21988	.07100	1.12434	.09366	0
Ethylene	18.3191	1.00100	15.7527	2.52638	0
Ethane	1.30647	.06499	1.04518	.26129	0
Propylene	6.67298	.24510	5.71941	.95356	0
Benzene	.98196	1.90487E-2	.90644	.07551	0
Paraffins	51.2432	1.24369	43.9206	7.32266	0
Olefins	1.37282	4.13054E-2	1.17665	.19617	0
HCN	-5.13848E-2	-2.87964E-3	-2.28354E-2	-1.90123E-3	0
Ammonia	1.25901E-2	1.12059E-3	0	2.22215E-3	0
COS	5.63488E-4	1.42102E-5	1.12697E-4	0	1.50282E-4
CS2	-3.78881E-2	-7.54322E-4	-5.98254E-3	0	0
SO2	5.36348E-2	1.26804E-3	0	0	2.68174E-2
Water	.37039	2.15553E-2	0	4.11505E-2	.32924
Other	0	96.0157	0	0	0
Gas Total:	96.0552	100	76.8495	18.2006	1.00321

TABLE A-67

PYROLYSIS SUMMARY REPORT — USARUN 72

RUN CONDITIONS

6330 mg. NO COAL
0 sec. 0 0 Amps
0 sec. 0 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
268 mm. Final Pressure for 100.193 liters

Butane 1300°C with H2
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	.13902
Tar	.33175
Gas	96.1136
Water	.97801
Missing	2.43759

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	17.7567	1.60156	13.3175	4.43917	0
CO	1.89115	.10366	.81055	0	1.08060
Hydrogen	6.02843	4.27864	0	6.02843	0
CO2	1.67208E-4	5.83262E-6	4.55977E-5	0	1.21610E-4
Acetylene	4.73617	.37280	4.37196	.36421	0
Ethylene	38.4107	2.09200	32.9218	5.48889	0
Ethane	1.50854	.07677	1.20051	.30012	0
Propylene	6.66982	.24505	5.71620	.95311	0
Benzene	4.90898	.09659	4.53148	.37750	0
Paraffins	11.5971	.28179	9.93992	1.65723	0
Olefins	2.61295	.07859	2.23956	.37339	0
HCN	.19060	1.08351E-2	.08470	7.05251E-3	0
Ammonia	2.59046E-2	2.33876E-3	0	4.57216E-3	0
COS	2.38445E-3	6.09952E-5	4.76891E-4	0	6.35934E-4
CS2	-6.54509E-4	-1.32178E-5	-1.03347E-4	0	0
SO2	-.08091	-1.94043E-3	0	0	-4.04568E-2
Water	.97801	5.77336E-2	0	.10865	.86935
Other	0	96.0913	0	0	0
Gas Total:	97.0916	100	75.1352	20.1023	1.91026

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TABLF A-68

RUN CONDITIONS

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 11 - 12 - 85   9 : 55
Stored => 11 - 14 - 85   10 : 43

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
772 mm. Final Pressure for 102.120 liters

Butane 1300°C with H2
Injector 36 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	.38546
Tar	2.54976
Gas	95.3388
Water	.51898
Missing	1.20695

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	22.7709	1.98795	17.0781	5.69273	0
CO	2.24640	.11898	.96281	0	1.28359
Hydrogen	7.12796	4.96398	0	7.12796	0
CO2	.84049	2.83291E-2	.22920	0	.61129
Acetylene	10.7898	.60800	9.96014	.82974	0
Ethylene	36.8657	1.96994	31.5976	5.26811	0
Ethane	1.25368	6.19752E-2	1.00295	.25073	0
Propylene	2.02527	.07300	1.73586	.28941	0
Benzene	9.23380	.17556	8.52372	.71007	0
Paraffins	.57819	1.37953E-2	.49557	.08262	0
Olefins	1.60663	4.73963E-2	1.37704	.22958	0
HCN	.78211	4.29594E-2	.34757	2.89383E-2	0
Ammonia	2.55935E-2	2.23270E-3	0	4.51726E-3	0
COS	1.32194E-3	3.26747E-5	2.64389E-4	0	3.52562E-4
CS2	7.21664E-3	1.40822E-4	1.13950E-3	0	0
SO2	-.09017	-2.08967E-3	0	0	-4.50897E-2
Water	.51898	2.96028E-2	0	5.76595E-2	.46132
Other	0	95.8050	0	0	0
Gas Total:	95.8578	100	73.3121	20.5721	2.31148

TABLE A-69

	Gas Scans =>	0 - 0 - 76	0 : 0
	Analysis =>	11 - 6 - 85	11 : 42
	Stored =>	11 - 6 - 85	12 : 31

RUN CONDITIONS

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
748.300 mm. Final Pressure for 113.681 liters

Butane 1300°C with H2
Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	4.42812
Tar	1.62717
Gas	91.6811
Water	.35834
Missing	1.90521

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	22.4107	1.74702	16.8080	5.60268	0
CO	2.22328	.10950	.95290	0	1.27038
Hydrogen	9.30015	5.81905	0	9.30015	0
CO2	.12093	1.44120E-2	.12539	0	.33443
Acetylene	16.0600	.81300	14.8250	1.23501	0
Ethylene	28.7693	1.38099	24.6582	4.11114	0
Ethane	.42518	1.95452E-2	.34015	.08503	0
Propylene	.30331	9.79553E-3	.25997	4.33440E-2	0
Benzene	10.7633	.19029	9.93563	.82770	0
Paraffins	0	0	0	0	0
Olefins	1.32385	3.51062E-2	1.13467	.18917	0
HCN	1.19450	6.10105E-2	.53083	4.41966E-2	0
Ammonia	1.99080E-2	1.61496E-3	0	3.51377E-3	0
COS	1.20440E-3	2.76823E-5	2.40881E-4	0	3.21215E-4
CS2	1.15925E-2	2.10351E-4	1.83046E-3	0	0
SO2	-5.63660E-2	-1.21886E-3	0	0	-2.82830E-2
Water	.35834	1.90068E-2	0	3.98122E-2	.31853
Other	0	91.3971	0	0	0
Gas Total:	92.0394	100	69.5729	21.4817	1.89539

PYROLYSIS SUMMARY REPORT   -   USARUN 71

Gas Scans =>	0 - 0 - 76	0 : 0
Analysis =>	11 - 18 - 85	11 : 40
Stored =>	11 - 19 - 85	4 : 44

RUN CONDITIONS

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
770 mm. Final Pressure for 100.193 liters

Butane 1300°C with H2
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	7.34597
Tar	2.50394
Gas	81.2889
Water	.99387
Missing	7.86729

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	19.6334	1.74701	14.7251	4.90837	0
CO	2.23777	.12234	.95911	0	1.27866
Hydrogen	9.33491	6.62597	0	9.......	0
CO2	6.69393E-3	2.32893E-4	1.82543E-3	0	4.86849E-3
Acetylene	19.2385	1.10500	17.7591	1.47944	0
Ethylene	19.9952	1.08900	17.1379	2.85732	0
Ethane	2.75124E-4	1.40390E-5	2.30099E-4	5.50249E-5	0
Propylene	1.31034	4.77600E-2	1.12309	.18724	0
Benzene	8.67374	.17023	8.00673	.66701	0
Paraffins	0	0	0	0	0
Olefins	.85781	2.58051E-2	.73523	.12258	0
HCN	1.32500	.07512	.58803	4.90250E-2	0
Ammonia	1.61658E-2	1.45572E-3	0	2.85327E-3	0
COS	-1.10887E-3	-2.82916E-5	-2.21774E-4	0	-2.95735E-4
CS2	1.27716E-2	2.57254E-4	2.01665E-3	0	0
SO2	-2.94074E-2	-7.03406E-4	0	0	-1.47037E-2
Water	.99387	5.85176E-2	0	.11041	.88345
Other	0	95.4007	0	0	0
Gas Total:	82.2827	100	61.0390	19.7192	2.15190

TABLE A-71

RUN CONDITIONS

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
754 mm. Final Pressure for 102.120 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 11 - 7 - 85   11 : 6
Stored => 11 - 7 - 85   12 : 27

Butane 1300°C with H2
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	15.1437
Tar	2.12480
Gas	71.5441
Water	.55225
Missing	10.6350

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	14.2614	1.36258	10.6960	3.56535	0
CO	2.08241	.11369	.89252	0	1.18989
Hydrogen	12.0458	8.39005	0	12.0458	0
CO2	.17752	6.16792E-3	4.84123E-2	0	.12911
Acetylene	21.7567	1.22599	20.0836	1.67309	0
Ethylene	10.8546	.44737	9.30352	1.55113	0
Ethane	3.04586E-2	1.55206E-3	2.43669E-2	6.09172E-3	0
Propylene	.70293	2.55852E-2	.60248	.10045	0
Benzene	9.16823	.17968	8.46319	.70503	0
Paraffins	0	0	0	0	0
Olefins	.46445	1.27055E-2	.39808	.06637	0
HCN	1.38307	.07863	.61721	5.13884E-2	0
Ammonia	6.19976E-3	5.57503E-4	0	1.09425E-3	0
COS	-2.64799E-3	-6.74662E-5	-5.29598E-4	0	-7.06219E-4
CS2	1.27606E-2	2.56673E-4	2.01490E-3	0	0
SO2	-3.29775E-3	-7.87695E-5	0	0	-1.64887E-3
Water	.55225	3.24703E-2	0	6.13555E-2	.49089
Other	0	97.1050	0	0	0
Gas Total:	72.0963	100	51.1309	19.8271	1.80755

.IFP   PYROLYSIS SUMMARY REPORT   -   USARUN 80

RUN CONDITIONS

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
759 mm. Final Pressure for 100.194 liters

Butane 1300°C with O2
Injector 6 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

Dry Wt. %

	Dry Wt. %
Char	0
Tar	.52922
Gas	116.865
Water	19.8324
Missing	-37.2274

GAS COMPOSITION

	Dry Wt. %	Volume %	%C		
Methane	4.29595	.47203	3.67195	1.22398	0
CO	16.2243	.81949	6.95374	0	9.27058
Hydrogen	1.11848	.79446	0	1.11848	0
CO2	20.1827	.70760	5.50384	0	14.6799
Acetylene	2.81895	.11594	1.86369	.15525	0
Ethylene	15.1358	.76548	12.9729	2.16291	0
Ethane	1.46287	.06903	1.17030	.29252	0
Propylene	6.57977	.22134	5.63952	.94025	0
Benzene	1.64873	3.26075E-2	1.52195	.12678	0
Paraffins	45.9684	1.11725	39.3995	6.56888	0
Olefins	1.62243	4.87483E-2	1.39058	.23184	0
HCN	-2.92370E-2	-1.67044E-3	-1.29929E-2	-1.08127E-3	0
Ammonia	9.09271E-3	8.25552E-4	0	1.60574E-3	0
COS	-9.75966E-3	-2.50925E-4	-1.95193E-3	0	-2.60290E-3
CS2	.15451	3.13624E-3	2.43974E-2	0	0
SO2	6.07059E-2	1.46323E-3	0	0	3.03529E-2
Water	19.8324	1.17669	0	2.20338	17.6290
Other	0	94.9003	0	0	0
Gas Total:	136.698	100	80.0975	15.0248	41.6063

TABLE A-73

RUN CONDITIONS

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
759 mm. Final Pressure for 102.120 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 0 - 0 - 76   0 : 0
Stored => 12 - 19 - 85   9 : 32

Butane 1300°C with O2
Injector 16 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	.51974
Tar	.34755
Gas	123.572
Water	26.7432
Missing	-51.1832

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	9.91569	.93798	7.43677	2.47892	0
CO	21.3870	1.15607	9.16647	0	12.2205
Hydrogen	1.72195	1.19894	0	1.72195	0
CO2	22.4251	.77139	6.11532	0	16.3097
Acetylene	5.55458	.3135?	5.12736	.42714	0
Ethylene	29.7440	1.47562	25.4936	4.25042	0
Ethane	1.67316	.08441	1.33853	.33463	0
Propylene	8.57503	.28326	7.34966	1.22537	0
Benzene	5.97508	.11594	5.51560	.45948	0
Paraffins	14.2622	.33992	12.2241	2.03807	0
Olefins	2.33649	.06903	2.00260	.33388	0
HCN	.31031	1.73951E-2	.13790	1.14815E-2	0
Ammonia	2.58874E-2	2.30479E-3	0	4.56913E-3	0
COS	-8.26856E-3	-2.08579E-4	-1.65371E-3	0	-2.20522E-3
CS2	.24981	4.97514E-3	3.94465E-2	0	0
SO2	-4.20344E-2	-9.94071E-4	0	0	-2.10172E-2
Water	26.7432	1.55679	0	2.97116	23.7720
Other	0	92.7729	0	0	0
Gas Total:	150.315	100	81.9458	16.2571	52.2791

PYROLYSIS SUMMARY REPORT

USARUM 78

RUN CONDITIONS

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
759 mm. Final Pressure for 102.120 liters

Butane 1300°C with O2
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	2.08214
Tar	1.05055
Gas	116.575
Water	21.4178
Missing	-41.1263

GAS COMPOSITION
-- ------------

	Dry Wt. %	Volume %	%C	%H	%O
Methane	14.6033	1.38142	10.9525	3.65084	0
CO	26.8787	1.45292	11.5202	0	15.3585
Hydrogen	3.23538	2.25296	0	3.23538	0
CO2	19.3398	.66522	5.27370	0	14.0651
Acetylene	11.5587	.67500	10.7622	.89655	0
Ethylene	27.1911	1.45296	23.3055	3.88561	0
Ethane	.66170	3.33838E-2	.52936	.13234	0
Propylene	2.06477	.06811	1.76971	.29505	0
Benzene	8.75202	.16982	8.07899	.67303	0
Paraffins	.13064	3.10935E-3	.11197	1.86695E-2	0
Olefins	2.06161	6.08695E-2	1.76700	.29460	0
HCN	.93823	5.25942E-2	.41694	3.47145E-2	0
Ammonia	2.55616E-2	2.27579E-3	0	4.51163E-3	0
COS	-1.06823E-2	-2.69468E-4	-2.13647E-3	0	-2.84898E-3
CS2	.25898	5.15769E-3	4.88939E-2	0	0
SO2	-5.20169E-2	-1.23014E-3	0	0	-2.60084E-2
Water	21.4178	1.24679	0	2.37952	19.0383
Other	0	92.4502	0	0	0
Gas Total:	137.993	100	74.5269	15.5008	48.4331

TABLE A-75

RUN CONDITIONS

6330 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
760 mm. Final Pressure for 102.120 liters

Butane 1300°C with O2
Injector 36 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	4.28436
Tar	1.94312
Gas	113.454
Water	23.0056
Missing	-42.6872

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	15.0329	1.41539	11.2746	3.75823	0
CO	30.8537	1.65998	13.2239	0	17.6298
Hydrogen	5.25197	4.00605	0	5.75197	0
CO2	18.6168	.63739	5.07692	0	13.5400
Acetylene	15.2432	.85894	14.0710	1.17220	0
Ethylene	12.1421	.91599	14.6925	2.44961	0
Ethane	3.99736E-3	2.00728E-4	3.19789E-3	7.99473E-4	0
Propylene	1.40327	5.03327E-2	1.20275	.20052	0
Benzene	8.46740	.16353	7.81626	.65114	0
Paraffins	0	0	0	0	0
Olefins	.93838	2.76973E-2	.80429	.13409	0
HCN	1.23891	.06912	.55057	4.58397E-2	0
Ammonia	1.74265E-2	1.54425E-3	0	3.07578E-3	0
COS	-1.52375E-2	-3.82577E-4	-3.04759E-3	0	-4.06385E-3
CS2	.23277	4.61409E-3	3.67558E-2	0	0
SO2	-1.80108E-2	-4.23945E-4	0	0	-9.00542E-3
Water	23.0056	1.33295	0	2.55592	20.4496
Other	0	93.1234	0	0	0
Gas Total:	136.459	100	68.7498	16.7234	51.6065

PYROLYSIS SUMMARY REPORT   -   USARUN 81

RUN CONDITIONS

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
767 mm. Final Pressure for 102.120 liters

Butane 1300°C with O2
Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	12.2796
Tar	2.39336
Gas	104.645
Water	14.7700
Missing	-34.0884

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	11.1812	1.03257	8.38592	2.79530	0
CO	33.3378	1.75925	14.2886	0	19.0492
Hydrogen	7.48183	5.21512	0	7.48183	0
CO2	18.8489	.63297	5.14010	0	13.7088
Acetylene	19.0410	1.07301	17.5768	1.46425	0
Ethylene	5.30923	.33294	5.40764	.90158	0
Ethane	6.88955E-4	3.39328E-5	5.51164E-4	1.37791E-4	0
Propylene	.54384	1.91327E-2	.46613	.07771	0
Benzene	7.21601	.13669	6.66109	.55491	0
Paraffins	.10236	2.43807E-3	.08774	1.46286E-2	0
Olefins	.58562	1.72099E-2	.50193	.08368	0
HCN	1.68479	.09220	.74872	6.23375E-2	0
Ammonia	6.75068E-3	5.86744E-4	0	1.19149E-3	0
COS	-1.86188E-2	-4.58512E-4	-3.72376E-3	0	-4.96564E-3
CS2	.18869	3.66860E-3	2.97952E-2	0	0
SO2	1.54947E-2	3.57728E-4	0	0	7.74735E-3
Water	14.7700	.83938	0	1.64095	13.1291
Other	0	94.6580	0	0	0
Gas Total:	119.415	100	59.2913	15.0785	45.8899

RUN CONDITIONS

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 102.120 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 12 - 18 - 85   12 : 18
Stored => 12 - 18 - 85   13 : 30

Butane 1300°C with O2
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	20.7867
Tar	1.68404
Gas	97.0980
Water	20.3268
Missing	-39.8957

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	8.53665	.75165	6.47748	2.15916	0
CO	33.7890	1.81278	14.4820	0	19.3070
Hydrogen	8.96582	6.24534	0	8.96582	0
CO2	18.9407	.64665	5.16514	0	13.7756
Acetylene	15.7409	.38639	14.5304	1.21047	0
Ethylene	2.97643	.15968	2.55114	.42534	0
Ethane	6.72906E-4	3.85901E-5	4.88725E-4	1.22181E-4	0
Propylene	.25600	9.15654E-3	.21942	3.65834E-2	0
Benzene	7.55415	.14548	6.97324	.58091	0
Paraffins	0	0	0	0	0
Olefins	.23206	6.85601E-3	.19898	3.31627E-2	0
HCN	1.05514	5.87055E-2	.46890	3.90485E-2	0
Ammonia	5.14481E-3	4.54621E-4	0	9.08059E-4	0
COS	-1.85014E-2	-4.63216E-4	-3.70029E-3	0	-4.93434E-3
CS2	.24258	4.79487E-3	3.83039E-2	0	0
SO2	2.81962E-2	6.61820E-4	0	0	1.40981E-2
Water	20.3268	1.17442	0	2.25831	18.0685
Other	0	94.6932	0	0	0
Gas Total:	112.424	100	51.1017	15.7108	51.1604

TABLE A-78

RUN CONDITIONS

6330 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
758 mm. Final Pressure for 105.974 liters

Gas Scans =) 0 - 0 - 76   0 : 0
Analysis =) 12 - 16 - 85   14 : 55
Stored =) 12 - 16 - 85   16 : 16

Butane 1300°C with O2
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	27.6255
Tar	1.33491
Gas	97.1647
Water	19.7230
Missing	-45.8483

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	8.87791	.81034	6.65843	2.21947	0
CO	39.3271	2.05121	16.8556	0	22.4715
Hydrogen	10.4423	7.01846	0	10.4423	0
CO2	15.5087	.51807	4.25651	0	11.3522
Acetylene	13.6734	.75329	12.8038	1.06663	0
Ethylene	2.07946	.10845	1.78231	.29715	0
Ethane	7.03320E-2	7.0332E-4	1.15581E-2	2.38953E-3	0
Propylene	.20960	7.29030E-3	.17970	2.99606E-2	0
Benzene	6.71582	.12574	6.19937	.51644	0
Paraffins	0	0	0	0	0
Olefins	1.83254E-2	5.21899E-4	1.57067E-2	2.61870E-3	0
HCN	1.06314	5.75048E-2	.47246	3.93363E-2	0
Ammonia	1.01819E-2	8.74702E-4	0	1.79712E-3	0
COS	-1.88226E-2	-4.58147E-4	-3.76453E-3	0	-5.02000E-3
CS2	.19992	3.84177E-3	3.15683E-2	0	0
SO2	2.26363E-2	5.16538E-4	0	0	1.13181E-2
Water	19.7230	1.10784	0	2.19123	17.5318
Other	0	94.8586	0	0	0
Gas Total:	116.887	100	49.2633	16.8998	51.3619

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TABLE A-79

```
                                    Gas Scans =>  0   0 - 70     0 : 0
RUN CONDITIONS                      Analysis =>  8 - 13 - 86    9 : 58
---------------                     Stored =>    8 - 13 - 86   10 : 25

  1440 mq. OXTRAP COAL
  0 sec. @ 0 Amps
  0 sec. @ 0 Amps
  1300 Degrees c. @ 0 torr with ALTUBE grid
  762 mm. Final Pressure for 88.6330 liters
```

Acetylene 1300°C "cleaned"
Injector 6 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	3.47222E-2
Tar	3.63194
Gas	88.1735
Water	2.03483
Missing	6.12500

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.13705	3.43041E-3	.10279	3.42644E-2	0
CO	.98101	1.40307E-2	.42046	0	.56065
Hydrogen	1.22915	.24146	0	1.22915	0
CO2	.79656	8.52231E-3	.25534	0	.68102
Acetylene	84.5416	1.26771	78.0404	6.50125	0
Ethylene	.02448	1.36421E-3	.06377	1.86330E-2	0
Ethane	2.05125E-4	3.15172E-6	1.88384E-4	4.72219E-5	0
Propylene	0	0	0	0	0
Benzene	.07481	3.84116E-4	.06706	5.75334E-3	0
Paraffins	0	0	0	0	0
Olefins	0	0	0	0	0
HCN	0	0	0	0	0
Ammonia	-7.71866E-4	-1.81826E-5	0	-1.36234E-4	0
COS	-4.58777E-3	-3.06206E-5	-9.17555E-4	0	-1.22356E-3
CS2	.06811	3.58890E-4	1.07546E-2	0	0
SO2	.12731	7.96642E-4	0	0	.06365
Water	2.03483	3.13414E-2	0	.22607	1.80876
Other	0	98.9282	0	0	0
Gas Total:	90.2083	100	78.9618	8.00705	3.11277

TABLE A-80

RUN CONDITIONS

1474 mq. COTRAP COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
763 mm. Final Pressure for 88.6330 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 7 - 18 - 86   10 : 7
Stored => 7 - 18 - 86   10 : 34

Acetylene 1300°C "cleaned"
Injector 16 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	1.26187
Tar	3.00542
Gas	96.2123
Water	1.66414
Missing	-2.14382

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.19117	4.85888E-3	.14337	4.77928E-2	0
CO	2.23898	3.19798E-2	.95955	0	1.27925
Hydrogen	1.85210	.36959	0	1.85210	0
CO2	2.85451	2.63832E-2	.77845	0	2.07616
Acetylene	87.3134	1.33992	80.5990	6.71440	0
Ethylene	.25370	3.38757E-3	.21762	3.62835E-2	0
Ethane	5.33430E-2	7.29864E-4	4.33744E-2	1.07686E-2	0
Propylene	3.61772E-2	3.50283E-4	3.10075E-2	5.16972E-3	0
Benzene	1.25508	6.42201E-3	1.15857	.09651	0
Paraffins	0	0	0	0	0
Olefins	0	0	0	0	0
HCN	0	0	0	0	0
Ammonia	1.58713E-4	3.79663E-6	0	2.80129E-5	0
COS	-6.43745E-3	-4.36310E-5	-1.28749E-3	0	-1.71686E-3
CS2	.08796	4.70671E-4	1.38893E-2	0	0
SO2	.07777	4.94183E-4	0	0	3.88870E-2
Water	1.66414	2.60286E-2	0	.18488	1.47925
Other	0	92.6511	0	0	0
Gas Total:	97.8765	100	83.9432	8.94795	4.87184

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TABLE A-81

RUN CONDITIONS

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 6 - 23 - 86   32 : 6
Stored => 6 - 23 - 86   32 : 24

1474 mg. COTRAP COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
752 mm. Final Pressure for 88.6330 liters

Acetylene 1300°C "cleaned"
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	4.51153
Tar	3.94165
Gas	89.4315
Water	.59556
Missing	1.51967

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
methane	.11533	2.65957E-3	.08649	2.88331E-2	0
CO	4.97954	.07101	2.13427	0	2.84537
Hydrogen	.75385	.15026	0	.75385	0
CO2	.44097	3.98935E-3	.12025	0	.32072
Acetylene	74.3554	1.14095	68.6375	5.71793	0
Ethylene	1.95988	2.94212E-2	1.70553	.28435	0
Ethane	9.49637E-4	1.31053E-5	7.59750E-4	1.89937E-4	0
Propylene	..4668	2.43076E-3	.21136	3.52398E-2	0
Benzene	2.81546	1.43617E-2	2.59895	.21650	0
Paraffins	.32945	1.62369E-3	.28237	4.70789E-2	0
Olefins	3.35537	1.65368E-2	2.87589	.47948	0
HCN	0	0	0	0	0
Ammonia	1.28401E-2	3.12689E-4	0	2.26629E-3	0
COS	-3.02311E-3	-2.08590E-5	-6.04623E-4	0	-8.06265E-4
CS2	1.76968E-2	9.63988E-5	2.79432E-3	0	0
SO2	-4.79173E-3	-3.09957E-5	0	0	-2.39586E-3
Water	.59556	9.48292E-3	0	.06616	.52939
Other	0	99.6730	0	0	0
Gas Total:	90.0271	100	78.6556	7.63111	3.69228

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PYROLYSIS SUMMARY REPORT - USARUN 111

RUN CONDITIONS

Gas Scans =)	0 - 0 - 76	0 : 0
Analysis =)	6 - 25 - 86	31 : 33
Stored =)	8 - 14 - 86	7 : 19

1441 mg. COTRAP COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 89.5960 liters

Acetylene 1300°C "cleaned"
Injector 36 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	11.0548
Tar	3.79597
Gas	85.6491
Water	1.72075
Missing	-2.22068

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.19767	4.89739E-3	.14825	4.94185E-2	0
CO	6.44774	.09128	2.76350	0	3.68424
Hydrogen	6.10687	1.17833	0	6.10687	0
CO2	.68702	5.94451E-3	.18735	0	.49967
Acetylene	67.5919	1.00396	62.3941	5.19782	0
Ethylene	.26254	3.71699E-3	.22502	3.75177E-2	0
Ethane	5.56245E-2	7.35648E-4	4.45396E-2	1.11349E-2	0
Propylene	3.74077E-2	3.53059E-4	3.20622E-2	5.34557E-3	0
Benzene	4.53157	2.24570	4.18309	.34847	0
Paraffins	0	0	0	0	0
Olefins	0	0	0	0	0
HCN	0	0	0	0	0
Ammonia	1.64112E-4	3.82672E-6	0	2.89658E-5	0
COS	-6.65641E-3	-4.39769E-5	-1.33128E-3	0	-1.77526E-3
CS2	.09095	4.74402E-4	1.43617E-2	0	0
SO2	.08041	4.98100E-4	0	0	4.02097E-2
Water	1.72075	2.62349E-2	0	.19117	1.52957
Other	0	92.5928	0	0	0
Gas Total:	87.3698	100	69.9969	11.9477	5.75192

TABLE A-83

Gas Scans => 4 - 4 - 76   0 : 0
Analysis => 8 - 8 - 76   0 : 0
Stored => 6 - 23 - 86   16 : 14

RUN CONDITIONS

1389.20 mq. COTRAP COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 86.7060 liters

Acetylene 1300°C "cleaned"
Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	34.5270
Tar	4.43420
Gas	58.7858
Water	5.41653
Missing	-3.16369

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.22007	5.44976E-3	.16505	5.50188E-2	0
CO	7.41913	.10498	3.17984	0	4.23929
Hydrogen	1.80629	.34874	0	1.80629	0
CO2	.45069	4.00264E-3	.12563	0	.33506
Acetylene	44.4140	.65653	40.9986	3.41544	0
Ethylene	.39432	5.57990E-3	.33797	5.55496E-2	0
Ethane	1.84615E-4	2.43821E-6	1.47692E-4	3.69230E-5	0
Propylene	5.43015E-2	5.12257E-4	4.65418E-2	7.75968E-3	0
Benzene	4.06708	2.00792E-2	3.75432	.31275	0
Paraffins	0	0	0	0	0
Olefins	-1.29258	-6.09684E-3	-1.10787	-.18471	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	-6.36478E-3	-4.20298E-5	-1.27295E-3	0	-1.69748E-3
CS2	.13436	7.00462E-4	2.12155E-2	0	0
SO2	5.76325E-2	3.56790E-4	0	0	2.88162E-2
Water	5.41653	.08254	0	.60177	4.81476
Other	0	99.2075	0	0	0
Gas Total:	64.2024	100	47.5202	6.07122	9.41623

TABLE A-84

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 6 - 25 - 86   ⁸0 : 10
Stored => 6 - 25 - 86   8 : 51

RUN CONDITIONS

1496 mg. COTRAP COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
748 mm. Final Pressure for 86.7060 liters

Acetylene 1300°C "cleaned"
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	34.9598
Tar	3.04144
Gas	49.9903
Water	3.71954
Missing	8.28877

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.24389	6.56029E-3	.18292	6.09742E-2	0
CO	6.50717	.10001	2.78997	0	3.71819
Hydrogen	7.01971	1.45187	0	7.01971	0
CO2	.42780	4.01069E-3	.11666	0	.31114
Acetylene	33.2887	.52941	30.7288	2.55990	0
Ethylene	.26502	4.07344E-3	.22715	3.78718E-2	0
Ethane	1.73648E-2	2.49107E-4	1.39918E-2	3.47297E-3	0
Propylene	.08590	8.80272E-4	.07363	1.22761E-2	0
Benzene	1.97860	1.87165	1.82645	.15215	0
Paraffins	0	0	0	0	0
Olefins	-.73732	-3.77757E-3	-.63195	-.10536	0
HCN	0	0	0	0	0
Ammonia	1.93206E-3	4.89112E-5	0	3.41008E-4	0
COS	-4.57351E-3	-3.28046E-5	-9.14703E-4	0	-1.21975E-3
CS2	.09831	5.56719E-4	1.55237E-2	0	0
SO2	4.01541E-2	2.70014E-4	0	0	2.00770E-2
Water	3.71954	6.15676E-2	0	.41324	3.30629
Other	0	99.2759	0	0	0
Gas Total:	53.7098	100	35.3412	10.1535	7.35449

TABLE A-85

```
                                       Gas Scans => 0 - 0 - 76    0 : 0
RUN CONDITIONS                         Analysis => 6 - 20 - 86    9 : 47
---------------                        Stored => 6 - 20 - 86    10 : 39

  1469 mg. COTRAP COAL
  0 sec. @ 0 Amps
  0 sec. @ 0 Amps
  1300 Degrees c. @ 0 torr with ALTUBE grid
  757 mm. Final Pressure for 86.7060 liters
```

Acetylene 1300°C "cleaned"
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	36.0789
Tar	2.79101
Gas	47.0425
Water	4.14871
Missing	9.93873

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.17969	4.68970E-3	.13477	4.49234E-2	0
CO	6.74153	.10053	2.88942	0	3.85211
Hydrogen	2.44383	.46499	0	2.44383	0
CO2	.46289	4.00264E-3	.12623	0	.33666
Acetylene	32.9475	.49084	30.4139	2.53366	0
Ethylene	.30658	4.57216E-3	.26277	4.38186E-2	0
Ethane	4.20528E-4	5.85059E-6	3.36262E-4	8.40657E-5	0
Propylene	.16645	1.65494E-3	.14266	2.37865E-2	0
Benzene	3.61470	1.75693E-2	3.33673	.27797	0
Paraffins	0	0	0	0	0
Olefins	-.76425	-3.79917E-3	-.65503	-.10921	0
HCN	1.77213	2.74072E-2	.78753	.06556	0
Ammonia	5.20052E-3	1.27741E-4	0	9.17893E-4	0
COS	-5.73235E-3	-3.98945E-5	-1.14647E-3	0	-1.52881E-3
CS2	.11218	6.16370E-4	1.77135E-2	0	0
SO2	3.36285E-2	2.19412E-4	0	0	1.68142E-2
Water	4.14871	.06663	0	.46092	3.68779
Other	6	99.4992	0	0	0
Gas Total:	51.1912	100	37.4559	5.78628	7.89185

A-87

TABLE A-86

	Gas Scans =>	0 - 0 - 76	0 : 0
RUN CONDITIONS	Analysis =>	7 - 1 - 85	14 : 10
---------------	Stored =>	7 - 1 - 85	14 : 11

2450 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1500 Degrees c. @ 0 torr with ALTUBE grid
756 mm. Final Pressure for 94.4132 liters

Acetylene 1500°C (contaminated)
Injector 16 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %

Char	19.2775
Tar	3.35102
Gas	51.3004
Water	9.23985
Missing	16.8310

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
	---------	---------			
Methane	.42725	1.70441E-2	.32043	.10681	0
CO	8.71544	.19867	3.73544	0	4.98000
Hydrogen	0	0	0	0	0
CO2	4.32894	.06279	1.18050	0	3.14844
Acetylene	25.5438	.62708	23.5795	1.96432	0
Ethylene	.72666	1.65649E-2	.62282	.10384	0
Ethane	7.56072E-4	1.60862E-5	6.04858E-4	1.51214E-4	0
Propylene	.09638	1.46471E-3	.08260	1.37728E-2	0
Benzene	7.14068	5.84329E-2	6.59157	.54911	0
Paraffins	0	0	0	0	0
Olefins	-.80318	-6.10305E-3	-.33840	-.11477	0
HCN	4.91811	.11626	2.18561	.18197	0
Ammonia	-1.87458E-4	-7.03829E-6	0	-3.30863E-5	0
COS	-8.50817E-3	-9.05102E-5	-1.70163E-3	0	-2.26913E-3
CS2	.13386	1.12429E-3	2.11380E-2	0	0
SO2	.08041	8.01958E-4	0	0	4.02058E-2
Water	9.23985	.22683	0	1.02654	8.21330
Other	0	98.6791	0	0	0
	---------	---------			
Gas Total:	60.5403	100	37.6301	3.83172	16.3796

TABLE A-87

RUN CONDITIONS

2450 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1500 Degrees c. @ 0 torr with ALTUBE grid
756 mm. Final Pressure for 102.120 liters

Gas Scans =) 0 - 0 - 76   0 : 0
Analysis =) 6 - 25 - 85   14 : 1
Stored =) 7 - 8 - 85   11 : 2

Acetylene 1500°C (contaminated)
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	45.0326
Tar	0
Gas	13.7537
Water	14.7645
Missing	26.4490

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.24366	8.95658E-3	.18274	6.09157E-2	0
CO	4.30142	.09034	1.84358	0	2.45783
Hydrogen	0	0	0	0	0
CO2	1.20586	1.61182E-2	.32583	0	.87702
Acetylene	6.57738	.15184	6.16382	.51348	0
Ethylene	.12888	2.52241E-3	.10292	1.71606E-2	0
Ethane	1.97729E-2	3.87635E-4	1.58183E-2	3.95459E-3	0
Propylene	.08510	1.19170E-3	.07294	1.21612E-2	0
Benzene	7.48245E-3	5.64186E-5	6.90705E-3	5.75400E-4	0
Paraffins	0	0	0	0	0
Olefins	-.31995	-2.24017E-3	-.27423	-4.57215E-2	0
HCN	1.11299	2.42438E-2	.49461	4.11807E-2	0
Ammonia	5.25155E-3	1.81682E-4	0	9.26900E-4	0
COS	-3.18980E-3	-3.12669E-5	-6.37961E-4	0	-8.50721E-4
CS2	.27605	2.13625E-3	4.35888E-2	0	0
SO2	2.19330E-2	2.01554E-4	0	0	1.09665E-2
Water	14.7645	.33397	0	1.64033	13.1241
Other	0	99.3712	0	0	0
Gas Total:	28.5183	100	8.98092	2.24497	16.4691

TABLE A-88

RUN CONDITIONS

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 6 - 20 - 85   15 : 24
Stored => 7 - 8 - 85   11 : 3

7350 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1500 Degrees c. @ 0 torr with ALTUBE grid
740 mm. Final Pressure for 95.3770 liters

Acetylene 1500°C (contaminated)
Injector 36 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	58.3442
Tar	0
Gas	15.2732
Water	.72660
Missing	25.6559

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.26658	3.25899E-2	.19994	.06664	0
CO	4.65418	.32512	1.99478	0	2.65939
Hydrogen	0	0	0	0	0
CO2	1.13084	5.02704E-2	.30838	0	.82246
Acetylene	5.20519	.39158	4.80491	.40027	0
Ethylene	.64583	4.51156E-2	.55354	.09228	0
Ethane	1.57391E-4	1.02618E-5	1.25913E-4	3.14783E-5	0
Propylene	.10469	4.87561E-3	.08973	1.49605E-2	0
Benzene	1.44700	3.62860E-2	1.33573	.11127	0
Paraffins	0	0	0	0	0
Olefins	.35288	8.21699E-3	.30245	5.04268E-2	0
HCN	1.43040	.10362	.63567	5.29250E-2	0
Ammonia	1.16378E-3	1.33902E-4	0	2.05408E-4	0
COS	-2.91396E-3	-9.49938E-5	-5.82792E-4	0	-7.77153E-4
CS2	1.77235E-2	4.56143E-4	2.79855E-3	0	0
SO2	1.94557E-2	5.94609E-4	0	0	9.72789E-3
Water	.72660	5.46620E-2	0	.08072	.64587
Other	0	98.9465	0	0	0
Gas Total:	15.9998	100	10.2274	.86976	4.13668

TABLE A-89

RUN CONDITIONS	Gas Scans => 0 - 0 - 76 0 : 0
--------------	Analysis => 6 - 31 - 85 14 : 8
	Stored => 7 - 8 - 85 11 : 5

2450 mg. ASIS COAL
0 sec. 0 0 Amps
0 sec. 0 0 Amps
1500 Degrees c. 0 0 torr with ALTUBE grid
758 mm. Final Pressure for 92.4864 liters

Acetylene 1500°C (contaminated)
Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %

Char	53.1102
Tar	0
Gas	18.6139
Water	8.59065
Missing	19.6852

GAS COMPOSITION
- -- ----------

	Dry Wt. %		Volume %	%C	%H	%O
	---------		--------			
Methane	.25561		1.04866E-2	.19171	.06390	0
CO	9.73818		.22829	4.17378	0	5.56439
Hydrogen	0		0	0	0	0
CO2	1.98134		2.95581E-2	.54031	0	1.44103
Acetylene	5.69526		.14379	5.25229	.43796	0
Ethylene	.12425		2.91285E-3	.10649	1.77557E-2	0
Ethane	1.57598E-2		3.44826E-4	1.26078E-2	3.15196E-3	0
Propylene	.10057		1.57180E-3	.08620	1.43717E-2	0
Benzene	1.50756E-2		1.26868E-4	1.39163E-2	1.15932E-3	0
Paraffins	0		0	0	0	0
Olefins	-.37199		-2.90691E-3	-.31883	-5.31585E-2	0
HCN	.85942		2.08937E-2	.38192	3.17988E-2	0
Ammonia	-2.11952E-3		-8.18387E-5	0	-3.74095E-4	0
COS	-7.83319E-3		-8.56954E-5	-1.56663E-3	0	-2.08911E-3
CS2	.19483		1.68272E-3	3.07636E-2	0	0
SO2	1.55515E-2		1.59501E-4	0	0	7.77578E-3
Water	8.59065		.21680	0	.95442	7.63623
Other	0		99.3463	0	0	0
	---------		--------			
Gas Total:	27.2045		100	10.4746	1.47099	14.6473

PYROLYSIS SUMMARY REPORT - USARUN 3

RUN CONDITIONS

2450 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1500 Degrees c. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 104.047 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 6 - 25 - 85   7 : 9
Stored => 7 - 8 - 85   11 : 6

Acetylene 1500°C (contaminated)
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	68.1061
Tar	0
Gas	15.3908
Water	9.58341
Missing	6.91961

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.15567	5.62794E-3	.11675	3.89196E-2	0
CO	4.23072	.08739	1.81328	0	2.41743
Hydrogen	0	0	0	0	0
CO2	.92683	1.21840E-2	.25274	0	.67408
Acetylene	7.31377	.16270	6.75134	.56242	0
Ethylene	.11195	2.31277E-3	.09595	1.59986E-2	0
Ethane	.12972	2.50120E-3	.10378	2.59453E-2	0
Propylene	2.72235E-2	3.74917E-4	2.33332E-2	3.89023E-3	0
Benzene	1.92222E-2	1.42544E-4	1.77440E-2	1.47818E-3	0
Paraffins	0	0	0	0	0
Olefins	-.36918	-2.54215E-3	-.31642	-5.27562E-2	0
HCN	2.66084	5.70027E-2	1.18247	.09845	0
Ammonia	-1.09635E-3	-3.73030E-5	0	-1.93507E-4	0
COS	-6.00467E-3	-5.78867E-5	-1.20093E-3	0	-1.60144E-3
CS2	.17343	1.31998E-3	2.73856E-2	0	0
SO2	1.77117E-2	1.60074E-4	0	0	8.85586E-3
Water	9.58341	.21320	0	1.06471	8.51869
Other	0	99.4577	0	0	0
Gas Total:	24.9742	100	10.0671	1.75888	11.6174

TABLE A-91

RUN CONDITIONS

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 6 - 21 - 85   14 : 59
Stored => 7 - 8 - 85   11 : 8

7350 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1500 Degrees c. @ 0 torr with ALTUBE grid
759 mm. Final Pressure for 105.974 liters

Acetylene 1500°C (contaminated)
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	76.7319
Tar	0
Gas	8.55114
Water	3.13329
Missing	11.5835

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.16134	1.73073E-2	.12100	4.03359E-2	0
CO	2.89438	.17741	1.24053	0	1.65385
Hydrogen	0	0	0	0	0
CO2	.29525	1.15172E-2	.08051	0	.21474
Acetylene	3.90918	.25805	3.60856	.30061	0
Ethylene	.30732	1.88380E-2	.26340	4.39166E-2	0
Ethane	1.00844E-2	5.76938E-4	8.06757E-3	2.01689E-3	0
Propylene	3.65890E-2	1.49519E-3	3.13604E-2	5.22857E-3	0
Benzene	8.99924E-3	1.98019E-4	8.30719E-3	6.92041E-4	0
Paraffins	0	0	0	0	0
Olefins	.17808	3.63861E-3	.15263	2.54478E-2	0
HCN	.68290	4.34101E-2	.30348	2.52673E-2	0
Ammonia	3.25710E-4	3.28836E-5	0	5.74879E-5	0
COS	-3.01526E-3	-8.62523E-5	-6.03052E-4	0	-8.04170E-4
CS2	6.07781E-2	1.37255E-3	9.59686E-3	0	0
SO2	8.90204E-3	2.38730E-4	0	0	4.45102E-3
Water	3.13329	.20683	0	.34810	2.78518
Other	0	99.2591	0	0	0
Gas Total:	11.6844	100	5.82687	.79160	4.65742

TABLE A-92

RUN CONDITIONS

Gas Scans =) 0 - 0 - 76   0 : 0
Analysis => 8 - 20 - 85   17 : 3
Stored => 8 - 23 - 85   23 : 46

2335 mg. ASIS COAL
0 sec. 0 0 Amps
0 sec. 0 0 Amps
1100 Degrees c. 0 0 torr with ALTUBE grid
758 mm. Final Pressure for 105.974 liters

Acetylene 1100°C (contaminated)
Injector 6 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	0
Tar	.98072
Gas	90.3954
Water	2.45247
Missing	6.17130

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.19475	6.55745E-3	.14606	4.86895E-2	0
CO	.14569	2.80318E-3	6.24456E-2	0	.08325
Hydrogen	0	0	0	0	0
CO2	.18240	2.23330E-3	4.97422E-2	0	.13266
Acetylene	89.7216	1.70184	82.8220	6.89959	0
Ethylene	4.87612E-2	9.38158E-4	4.17932E-2	6.96798E-3	0
Ethane	7.68272E-4	1.37960E-5	6.14618E-4	1.53654E-4	0
Propylene	1.88064E-2	2.41222E-4	1.61190E-2	2.68744E-3	0
Benzene	.07665	5.27704E-4	.07076	5.89511E-3	0
Paraffins	0	0	0	0	0
Olefins	0	-2.15172E-2	0	0	0
HCN	0	-.10145	0	0	0
Ammonia	0	1.64837E-5	0	0	0
COS	0	-3.05468E-5	0	0	0
CS2	0	2.13182E-4	0	0	0
SO2	0	1.99600E-3	0	0	0
Water	2.45247	5.08147E-2	0	.27246	2.18000
Other	0	94.0177	0	0	0
Gas Total:	92.8479	100	83.2095	7.23645	2.39591

A-94

TABLE A-93

RUN CONDITIONS

21## mg. ASIS COAL
sec. @ # Amps
sec. @ # Amps
11## Degrees c. @ # torr with ALTUBE grid
758 mm. Final Pressure for 1#5.974 liters

Acetylene 1100°C (contaminated)
Injector 16 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	#
Tar	1.64761
Gas	96.239#
Water	.95146
Missing	1.1619#

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.124#3	3.75598E-3	.#93#2	3.1##92E-2	#
CO	.69592	1.2#419E-2	.29827	#	.39765
Hydrogen	.68#95	.15197	#	.68#95	#
CO2	1.51126	1.6641#E-2	.41212	#	1.#9914
Acetylene	9#.8#95	1.55145	83.8262	6.98325	#
Ethylene	.#9535	1.65##5E-3	.#8173	1.36269E-2	#
Ethane	6.31976E-4	1.#2#63E-5	5.#558#E-4	1.26395E-4	#
Propylene	.#64#2	7.38616E-4	5.48792E-2	9.14973E-3	#
Benzene	2.238#9	1.38522E-2	2.#6598	.1721#	#
Paraffins	#	#	#	#	#
Olefins	#	-1.28762E-2	#	#	#
HCN	#	-.#952#	#	#	#
Ammonia	#	3.98125E-5	#	#	#
COS	#	-4.1#58#E-5	#	#	#
CS2	#	2.271#3E-4	#	#	#
SO2	#	1.75127E-3	#	#	#
Water	.95146	1.77301E-2	#	.1#57#	.84575
Other	#	97.6216	#	#	#
Gas Total:	97.19#4	1##	86.8328	7.99593	2.34255

TABLE A-94

RUN CONDITIONS

Gas Scans => # - # - 76   0 : 0
Analysis => 8 - 15 - 85   # : 24
Stored => 8 - 23 - 85   23 : 45

2100 mg. ASIS COAL
sec. @ # Amps
sec. @ # Amps
1100 Degrees c. @ # torr with ALTUBE grid
757 mm. Final Pressure for 109.827 liters

Acetylene 1100°C (contaminated)
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	.13333
Tar	4.11904
Gas	103.380
Water	#
Missing	-7.63333

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.40478	1.20024E-2	.30359	.10119	#
CO	4.01715	.06806	1.72175	#	2.29540
Hydrogen	.85238	.18295	#	.85238	#
CO2	6.36646	.06864	1.73613	#	4.63032
Acetylene	74.2380	1.22457	68.5291	5.70890	#
Ethylene	.92502	1.56732E-2	.79283	.13218	#
Ethane	.07035	1.11253E-3	5.62811E-2	1.40702E-2	#
Propylene	.38151	4.30950E-3	.32699	5.45187E-2	#
Benzene	15.3285	.09326	14.1498	1.17876	#
Paraffins	#	#	#	#	#
Olefins	.75660	4.27318E-3	.64848	.10811	#
HCN	#	.09359	#	#	#
Ammonia	#	5.95409E-5	#	#	#
COS	#	-4.86159E-5	#	#	#
CS2	#	2.00196E-3	#	#	#
SO2	#.	9.14485E-4	#	#	#
Water	#	.43457	#	#	#
Other	#	95.3218	#	#	#
Gas Total:	103.380	100	88.2650	8.15014	6.92572

PYROLYSIS SUMMARY REPORT - USARUN 22

RUN CONDITIONS

2100 mg. NO COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1100 Degrees c. @ 0 torr with ALTUBE grid
750 mm. Final Pressure for 105.974 liters

Acetylene 1100°C (contaminated)
Injector 36 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	.15714
Tar	2.86666
Gas	100.110
Water	3.46106
Missing	-6.59523

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.52718	1.60175E-2	.39538	.13179	0
CO	4.96605	.08621	2.12845	0	2.83760
Hydrogen	1.04285	.23205	0	1.04285	0
CO2	6.09535	.06734	1.66220	0	4.43315
Acetylene	65.7619	1.12269	60.7048	5.05709	0
Ethylene	.68150	1.18321E-2	.58411	.09738	0
Ethane	2.75752E-4	4.46838E-6	2.20602E-4	5.51505E-5	0
Propylene	.27065	3.13273E-3	.23198	3.86770E-2	0
Benzene	20.1761	.12572	18.6246	1.55154	0
Paraffins	0	0	0	0	0
Olefins	.55154	3.19193E-3	.47273	.07881	0
HCN	0	.10243	0	0	0
Ammonia	0	-8.82771E-5	0	0	0
COS	0	-5.91432E-5	0	0	0
CS2	0	3.96271E-5	0	0	0
SO2	0	6.99945E-4	0	0	0
Water	3.46106	.06471	0	.38452	3.07654
Other	0	98.8195	0	0	0
	---------	---------			
Gas Total:	103.571	100	84.8045	8.38275	10.3472

TABLE A-96

	Gas Scans =>	0 - 0 - 76	0 : 0
RUN CONDITIONS	Analysis =>	8 - 19 - 85	3 : 21
---------------	Stored =>	8 - 21 - 85	15 : 6

2100 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1100 Degrees c. @ 0 torr with ALTUBE grid
756 mm. Final Pressure for 105.974 liters

Acetylene 1100°C (contaminated)
Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	8.03333
Tar	1.52857
Gas	86.8095
Water	0
Missing	3.62857

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.57028	1.73728E-2	.42771	.14257	0
CO	5.89814	.10267	2.52794	0	3.37019
Hydrogen	1.45714	.29629	0	1.45714	0
CO2	5.26348	5.83068E-2	1.43535	0	3.82813
Acetylene	66.0476	1.12830	60.9685	5.07906	0
Ethylene	.98228	1.70992E-2	.84191	.14036	0
Ethane	5.43773E-4	8.83477E-6	4.35018E-4	1.08754E-4	0
Propylene	.18261	2.11930E-3	.15652	2.60961E-2	0
Benzene	6.27142	3.57142E-2	5.78915	.48227	0
Paraffins	0	0	0	0	0
Olefins	.14604	8.47454E-4	.12517	2.08703E-2	0
HCN	0	.09948	0	0	0
Ammonia	0	-3.76121E-5	0	0	0
COS	0	-4.71614E-5	0	0	0
CS2	0	1.61589E-3	0	0	0
SO2	0	7.75630E-4	0	0	0
Water	0	.18463	0	0	0
Other	0	98.5185	0	0	0
Gas Total:	86.8095	100	72.2727	7.34849	7.19832

TABLE A-97

RUN CONDITIONS

```
Gas Scans =>  0 - 0 - 76     0 : 0
Analysis =>  8 - 14 - 85     6 : 5
Stored =>  8 - 23 - 85    23 : 38
```

```
2275 mg. ASIS COAL
0 sec. 0 0 Amps
0 sec. 0 0 Amps
1100 Degrees c. 0 0 torr with ALTUBE grid
758 mm. Final Pressure for 115.608 liters
```

Acetylene 1100°C (contaminated)
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	12.7032
Tar	2.47472
Gas	93.8505
Water	0
Missing	-9.02857

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.70741	2.38377E-2	.59056	.19685	0
CO	5.33025	.09220	2.28454	0	3.04570
Hydrogen	1.34505	.29683	0	1.34505	0
CO2	4.95652	5.45638E-2	1.35164	0	3.60488
Acetylene	63.6483	1.68047	58.7537	4.89455	0
Ethylene	1.44033	2.49163E-2	1.23450	.20582	0
Ethane	2.97032E-4	4.79582E-6	2.37626E-4	5.94065E-5	0
Propylene	.16310	1.88107E-3	.13980	2.33081E-2	0
Benzene	15.5780	.09670	14.3800	1.19794	0
Paraffins	0	0	0	0	0
Olefins	.59617	3.43773E-3	.51097	.08519	0
HCN	0	.09219	0	0	0
Ammonia	0	1.63173E-4	0	0	0
COS	0	-5.18615E-5	0	0	0
CS2	0	1.43553E-3	0	0	0
SO2	0	6.83473E-4	0	0	0
Water	0	.16715	0	0	0
Other	0	98.5567	0	0	0
Gas Total:	93.8505	100	79.2461	7.94880	. 6.65058

PYROLYSIS SUMMARY REPORT - USARUN 20

RUN CONDITIONS

2170 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1100 Degrees c. @ 0 torr with ALTUBE grid
750 mm. Final Pressure for 109.827 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 8 - 19 - 85   12 : 34
Stored => 8 - 23 - 85   23 : 36

Acetylene 1100°C (contaminated)
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	12.9124
Tar	3.91705
Gas	80.3917
Water	0
Missing	2.77880

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.30679	9.32543E-3	.23009	.07669	0
CO	5.51372	.09576	2.36318	0	3.15054
Hydrogen	1.57142	.34960	0	1.57142	0
CO2	4.52558	5.00218E-2	1.23412	0	3.29146
Acetylene	56.7741	.96701	52.4082	4.36593	0
Ethylene	.73349	1.27401E-2	.62867	.10481	0
Ethane	4.07978E-4	6.61382E-6	3.26382E-4	8.15956E-5	0
Propylene	.14427	1.67057E-3	.12365	2.06162E-2	0
Benzene	10.8202	.06746	9.98819	.83207	0
Paraffins	0	0	0	0	0
Olefins	0	-3.12500E-3	0	0	0
HCN	0	.07690	0	0	0
Ammonia	0	1.16555E-4	0	0	0
COS	0	-6.57651E-5	0	0	0
CS2	0	2.56201E-3	0	0	0
SO2	0	6.80951E-4	0	0	0
Water	0	.43761	0	0	0
Other	0	98.5625	0	0	0
Gas Total:	80.3917	100	66.9765	6.97165	6.44200

PYROLYSIS SUMMARY REPORT -- USARUN 96

RUN CONDITIONS

1800 mg. DEGAS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees C. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 90.5596 liters

Benzene 1300°C
Injector 6 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	.98333
Tar	1.04444
Gas	64.8007
Water	5.08814
Missing	28.0833

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	7.26319E-4	2.22385E-5	5.44739E-4	1.81579E-4	0
CO	.52166	9.12708E-3	.22358	0	.29887
Hydrogen	0	0	0	0	0
CO2	.63613	7.08263E-3	.17347	0	.46266
Acetylene	5.28447E-2	9.95695E-4	4.97810E-2	4.05376E-3	0
Ethylene	1.99862E-2	3.47931E-4	1.70445E-2	2.84174E-3	0
Ethane	3.18720E-3	5.28459E-5	2.54976E-3	6.37441E-4	0
Propylene	-6.08042E-2	-7.89222E-4	-5.21153E-2	-8.68892E-3	0
Benzene	59.0555	.36063	54.5141	4.54137	0
Paraffins	.83983	4.89795E-3	.71982	.12001	0
Olefins	3.51001	2.04704E-2	3.00843	.50158	0
HCN	-.24557	-4.45200E-3	-.18904	-9.07869E-3	0
Ammonia	3.04119E-3	8.76381E-5	0	5.36720E-4	0
COS	-4.18172E-3	-3.41430E-5	-8.36344E-4	0	-1.11526E-3
CS2	.08254	5.32077E-4	1.30338E-2	0	0
SO2	1.06095E-2	8.12113E-5	0	0	5.30479E-3
Water	5.08814	.09587	0	.56529	4.52284
Other	0	99.1494	0	0	0
Gas Total:	69.8888	100	58.5594	5.71875	5.28777

TABLE A-100

RUN CONDITIONS

```
                                      Gas Scans =>  0 - 0 - 76     0 : 0
                                      Analysis =>   5 - 23 - 86    9 : 42
                                      Stored =>     5 - 23 - 86    9 : 50
```

1833 mg. DEGAS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
758 mm. Final Pressure for 94.4130 liters

Benzene 1300°C
Injector 16 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	4.58810
Tar	2.27495
Gas	92.0194
Water	5.20914
Missing	-4.09165

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	7.43592E-4	2.22834E-5	5.57694E-4	1.85898E-4	0
CO	.53407	9.14553E-3	.22890	0	.30516
Hydrogen	0	0	0	0	0
CO2	.65126	7.09694E-3	.17759	0	.47366
Acetylene	5.41014E-2	9.97707E-4	4.99410E-2	4.16040E-3	0
Ethylene	2.03592E-2	3.48634E-4	1.74498E-2	2.90933E-3	0
Ethane	3.26300E-3	5.21511E-5	2.61840E-3	6.52500E-4	0
Propylene	-6.22502E-2	-7.10655E-4	-5.33547E-2	-8.89556E-3	0
Benzene	86.5248	.51596	79.8710	6.65375	0
Paraffins	.85981	4.90784E-3	.73694	.12286	0
Olefins	3.59340	2.05118E-2	3.07997	.51350	0
HCN	-.25120	-4.46100E-3	-.11163	-9.29459E-3	0
Ammonia	3.11351E-3	8.78152E-5	0	5.49536E-4	0
COS	-4.28117E-3	-3.42120E-5	-8.56234E-4	0	-1.14178E-3
CS2	.08450	5.33153E-4	1.33438E-2	0	0
SO2	1.08619E-2	8.13754E-5	0	0	5.43095E-3
Water	5.20914	.09606	0	.57873	4.63040
Other	0	99.1386	0	0	0
Gas Total:	97.2285	100	84.0125	7.85913	5.41353

TABLE A-101

PYROLYSIS SUMMARY REPORT - TISARUN 72

RUN CONDITIONS

Gas Scans =) 0 - 0 - 76   0 : 0
Analysis =) 0 - 0 - 76   0 : 0
Stored =) 5 - 22 - 86   15 : 15

1831 mg. DEGAS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
757 mm. Final Pressure for 91.5230 liters

Benzene 1300°C
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	18.7329
Tar	6.84325
Gas	70.4085
Water	3.69142
Missing	.32386

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.24030	7.19947E-3	.18022	6.00764E-2	0
CO	4.89796	.07264	1.75634	0	2.34151
Hydrogen	1.82676	.24792	0	1.02676	0
CO2	.55151	5.99735E-3	.15042	0	.40118
Acetylene	.51784	2.00132E-3	.34286	2.89292E-2	0
Ethylene	.86506	1.11807E-3	5.40565E-2	9.21257E-3	0
Ethane	5.17672E-4	5.1234E-6	2.50138E-4	6.25345E-5	0
Propylene	1.66351E-2	1.96603E-4	1.42579E-2	2.37716E-3	0
Benzene	61.3326	.37648	56.6161	4.71647	0
Paraffins	.42334	2.50164E-3	.36284	6.04956E-2	0
Olefins	2.17522	1.28539E-2	1.86438	.31083	0
HCN	-.11300	-2.07757E-3	-5.02204E-2	-4.18127E-3	0
Ammonia	1.35022E-2	3.94249E-4	0	2.38315E-3	0
COS	-7.21600E-3	-5.96979E-5	-1.44320E-3	0	-1.92450E-3
CS2	.09208	6.01456E-4	1.45407E-2	0	0
SO2	8.06260E-3	6.25329E-5	0	0	4.03130E-3
Water	3.69142	.07047	0	.41011	3.28130
Other	0	99.5007	0	0	0
Gas Total:	74.0999	100	61.3096	6.62340	6.02612

TABLE A-102

RUN CONDITIONS
....

1700 mq. DEGAS COAL
0 sec. @ 0 Amps
0 sec. 9 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
759 mm. Final Pressure for 94.4130 liters

Benzene 1300°C
Injector 36 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	37.6117
Tar	5.18823
Gas	44.7907
Water	6.00922
Missing	6.40000

GAS COMPOSITION
....

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.46020	1.27310E-2	.34515	.11505	0
CO	5.39196	.08523	2.31099	0	3.08097
Hydrogen	2.76470	.59815	0	2.76470	0
CO2	.43836	4.40975E-3	.11954	0	.31882
Acetylene	.57823	9.84370E-3	.53376	4.44658E-2	0
Ethylene	.06371	1.00821E-3	5.46651E-2	9.11404E-3	0
Ethane	1.16968E-4	1.72575E-6	9.35750E-5	2.33937E-5	0
Propylene	-4.86966E-2	-5.13192E-4	-4.17378E-2	-6.95874E-3	0
Benzene	33.8941	.18748	31.2876	2.60645	0
Paraffins	.12133	6.39364E-4	.10399	1.73391E-2	0
Olefins	.94029	4.95470E-3	.80593	.13436	0
HCN	-.13946	-2.28626E-3	-6.19774E-2	-5.16013E-3	0
Ammonia	7.92945E-3	2.06455E-4	0	1.39954E-3	0
COS	-5.03872E-3	-3.71706E-5	-1.00774E-3	0	-1.34382E-3
CS2	.13817	8.04728E-4	2.18179E-2	0	0
SO2	6.81423E-3	4.71268E-5	0	0	3.40711E-3
Water	6.00922	.16230	0	.66762	5.34160
Other	0	99.6173	0	0	0
Gas Total:	50.8000	100	35.4789	6.34843	8.74346

TABLE A-103

RUN CONDITIONS

1800 mg. DEGAS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1320 Degrees c. @ 0 torr with ALTUBE grid
761 mm. Final Pressure for 90.5596 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 0 - 0 - 76   0 : 0
Stored => 5 - 22 - 86   14 : 57

Benzene 1300°C
Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	60.8888
Tar	3.58888
Gas	24.9989
Water	5.79554
Missing	4.92777

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.30000	8.93561E-3	.22500	.07500	0
CO	4.21458	.07360	1.80650	0	2.40838
Hydrogen	3.60555	.85939	0	3.60555	0
CO2	1.53622	1.70710E-2	.41892	0	1.11729
Acetylene	1.30555	2.40473E-2	1.20515	.10039	0
Ethylene	.09022	1.57548E-3	.07732	1.28927E-2	0
Ethane	1.81631E-4	2.96123E-6	1.45353E-4	3.53383E-5	0
Propylene	5.81818E-2	-6.27316E-4	-4.98669E-2	-8.31407E-3	0
Benzene	14.9222	.89119	13.7747	1.14751	0
Paraffins	2.22379E-2	1.29441E-4	1.90601E-2	3.17780E-3	0
Olefins	.38629	2.24854E-3	.33109	5.52018E-2	0
HCN	-.12453	-2.25524E-3	-5.53441E-2	-4.60785E-3	0
Ammonia	8.48661E-3	2.44087E-4	0	1.49788E-3	0
COS	-4.78846E-3	-3.90215E-5	-9.57692E-4	0	-1.27708E-3
CS2	.14189	9.12890E-4	2.24055E-2	0	0
SO2	7.94630E-3	6.07078E-5	0	0	3.97315E-3
Water	5.79554	.10898	0	.64388	5.15165
Other	0	99.6778	0	0	0
Gas Total:	30.7944	100	17.7741	5.63224	8.68003

TABLE A-104

RUN CONDITIONS

1742 mg. DEGAS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
760 mm. Final Pressure for 90.5596 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 5 - 22 - 86   16 : 14
Stored => 5 - 23 - 86   7 : 54

Benzene 1300°C
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	61.9977
Tar	2.93340
Gas	25.4926
Water	4.76795
Missing	4.80826

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%0
Methane	.58776	1.73475E-2	.44082	.14694	0
CO	3.57845	6.03521E-2	1.53372	0	2.04472
Hydrogen	3.88597	.87894	0	3.88597	0
CO2	.37887	3.99999E-3	.10331	0	.27555
Acetylene	2.50769	4.10526E-2	2.13023	.17746	0
Ethylene	.13418	2.25315E-3	.11501	1.21755E-2	0
Ethane	2.46429E-4	3.87906E-6	1.97143E-4	4.92858E-5	0
Propylene	-4.56286E-2	-5.13031E-4	-3.91082E-2	-6.52032E-3	0
Benzene	13.9613	.08452	12.8877	1.07362	0
Paraffins	.24291	1.36563E-3	.20820	3.47127E-2	0
Olefins	.20272	1.13965E-3	.17375	2.89687E-2	0
HCN	.14223	2.48762E-3	.06320	5.26252E-3	0
Ammonia	5.22133E-3	1.45040E-4	0	9.21565E-4	0
COS	-5.05288E-3	-3.97689E-5	-1.01057E-3	0	-1.34760E-3
CS2	.15020	9.33311E-4	2.37173E-2	0	0
SO2	6.38134E-3	4.70856E-5	0	0	3.19067E-3
Water	4.76795	.08639	0	.52971	4.23823
Other	0	99.7053	0	0	0
Gas Total:	30.2606	100	17.6397	5.81629	6.56035

TABLE A-105

RUN CONDITIONS

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 5 - 22 - 86   13 : 44
Stored => 5 - 22 - 86   14 : 1

1800 mg. DEGAS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
765 mm. Final Pressure for 90.5596 liters

Benzene 1300°C
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	76.3944
Tar	1.39444
Gas	25.5944
Water	3.19552
Missing	-7.07888

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	.68155	2.07039E-2	.51116	.17038	0
CO	4.04981	.07029	1.73574	0	2.31406
Hydrogen	4.94444	1.17955	0	4.94444	0
CO2	6.16079E-5	6.80539E-7	1.68004E-5	0	4.48074E-5
Acetylene	4.14444	.07601	3.82573	.31870	0
Ethylene	.16611	2.98358E-3	.14238	2.37385E-2	0
Ethane	4.24941E-4	6.88457E-6	3.39953E-4	8.49882E-5	0
Propylene	1.84788E-2	2.13842E-4	1.58382E-2	2.64062E-3	0
Benzene	10.9388	.06684	10.0976	.84120	0
Paraffins	.08301	4.80354E-4	.07115	1.18632E-2	0
Olefins	.27005	1.56255E-3	.23146	3.85903E-2	0
HCN	.18736	3.32278E-3	.08326	6.93241E-3	0
Ammonia	6.28446E-3	1.79675E-4	0	1.10920E-3	0
COS	-5.14632E-3	-4.16883E-5	-1.02926E-3	0	-1.37252E-3
CS2	.12224	7.81796E-4	1.93028E-2	0	0
SO2	5.27610E-3	4.00684E-5	0	0	2.63805E-3
Water	3.19552	5.97363E-2	0	.35502	2.84050
Other	0	99.7162	0	0	0
Gas Total:	28.7900	100	16.7330	6.71472	5.15587

PYROLYSIS SUMMARY REPORT -- USRRUN 188

RUN CONDITIONS

2580 mg. ASIS COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
761 mm. Final Pressure for 104.047 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 7 - 7 - 87   14 : 28
Stored => 5 - 22 - 86   26 : 35

Dodecane 1300°C
Injector 26 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	0
Tar	1.70542
Gas	94.6421
Water	3.76866
Missing	-.11627

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	10.0896	.38465	7.56722	2.52240	0
CO	1.65543	3.56275E-2	.70094	0	.93448
Hydrogen	1.39534	.40867	0	1.39534	0
CO2	.15583	1.99737E-3	4.22790E-2	0	.11275
Acetylene	7.06876	.16611	6.53625	.54451	0
Ethylene	41.6673	.90771	35.7131	5.95426	0
Ethane	2.68190	5.45296E-2	2.14552	.53638	0
Propylene	10.8527	.15374	9.30186	1.55085	0
Benzene	8.02967	.06279	7.41219	.61748	0
Paraffins	.65891	8.01576E-3	.56475	.09415	0
Olefins	10.3875	.12391	8.90320	1.48438	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	3.76866	.08841	0	.41869	3.34996
Other	0	97.1841	0	0	0
Gas Total:	98.4108	100	78.8873	15.1184	4.39721

TABLE A-107

RUN CONDITIONS

2700 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
753 mm. Final Pressure for 100.194 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 6 - 30 - 87   7 : 53
Stored => 11 - 18 - 87   9 : 7

Dodecane 1300°C
Injector 46 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	1.25925
Tar	8.14814
Gas	95.2725
Water	1.43120
Missing	-6.11111

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	10.8518	.43904	8.13888	2.71296	0
CO	0	.12098	2.57160	0	3.42840
Hydrogen	4.22222	1.36653	0	4.22222	0
CO2	.4073	5.97609E-3	.11109	0	.29610
Acetylene	1.72962	.43027	15.9662	1.33008	0
Ethylene	30	.69332	25.7130	4.28700	0
Ethane	.54599	1.22964E-2	.43759	.10939	0
Propylene	3.73527	5.99779E-2	3.20150	.53377	0
Benzene	11.2227	.09703	10.3596	.86302	0
Paraffins	4.29251	3.44628E-2	3.67911	.61339	0
Olefins	6.70370	5.28552E-2	5.74574	.95795	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	1.43120	3.71233E-2	0	.15900	1.27219
Other	0	98.9189	0	0	
Gas Total:	96.7037	100	75.9244	15.7888	4.99690

TABLE A-108

Gas Scans => 0 - 1 - 76   0 : 0
Analysis => 7 - 3 - 87   7 : 56
Stored => 7 - 7 - 87   18 : 8

RUN CONDITIONS

2750 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
755 mm. Final Pressure for 99.2300 liters

Dodecane 1300°C
Injector 56 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	15.4545
Tar	2.87272
Gas	65.4050
Water	4.63126
Missing	11.6363

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	10.1201	.43462	7.59011	2.53003	0
CO	5.17568	.12704	2.21872	0	2.95795
Hydrogen	8.76363	2.98993	0	8.76363	0
CO2	.12141	1.89686E-3	3.31086E-2	0	.08838
Acetylene	23.5272	.60264	21.7180	1.80924	0
Ethylene	7.03863	.17745	6.19754	1.03328	0
Ethane	2.43983E-2	5.58640E-4	1.95186E-2	4.87967E-3	0
Propylene	.44486	7.26512E-3	.38050	.06345	0
Benzene	9.43703	.08313	8.71132	.72570	0
Paraffins	0	0	0	0	0
Olefins	.54545	9.27152E-3	.46750	.07794	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	0	0	0	0	0
Water	4.63126	.12239	0	.51453	4.11673
Other	0	98.4747	0	0	0
Gas Total:	70.0363	100	47.3364	15.5227	7.16299

PYROLYSIS SUMMARY REPORT - USARUN 116

RUN CONDITIONS

2802 mg. DEOX COAL
0 sec. @ 0 Amps
0 sec. @ 0 Amps
1300 Degrees c. @ 0 torr with ALTUBE grid
753 mm. Final Pressure for 94.4130 liters

Gas Scans => 0 - 0 - 76   0 : 0
Analysis => 8 - 8 - 86   01 : 25
Stored => 11 - 16 - 87   11 : 44

Dodecane 1300°C
Injector 66 cm Above Extractor

PYROLYSIS PRODUCT DISTRIBUTION

	Dry Wt. %
Char	27.3733
Tar	1.93790
Gas	67.0288
Water	.70849
Missing	2.95146

GAS COMPOSITION

	Dry Wt. %	Volume %	%C	%H	%O
Methane	7.23411	.32139	5.42558	1.80852	0
CO	4.57720	.11577	1.87584	0	2.50216
Hydrogen	12.5445	4.52788	0	12.5445	0
CO2	6.28876E-4	1.05804E-5	1.71494E-4	0	4.57381E-4
Acetylene	27.3372	.76228	25.5455	2.14868	0
Ethylene	3.75161	.09918	3.21555	.53611	0
Ethane	3.49261E-4	8.51831E-6	2.79409E-4	6.98523E-5	0
Propylene	.25156	4.43392E-3	.21561	3.59482E-2	0
Benzene	3.88294	3.54581E-2	3.58434	.29859	0
Paraffins	.11823	1.04282E-3	.10134	1.68764E-2	0
Olefins	5.35706	4.72106E-2	4.59153	.76552	0
HCN	0	0	0	0	0
Ammonia	0	0	0	0	0
COS	0	0	0	0	0
CS2	0	0	0	0	0
SO2	2.66738E-2	0	0	0	1.33369E-2
Water	.70849	2.01722E-2	0	.07871	.62978
Other	0	98.7614	0	0	0
Gas Total:	67.7373	100	44.7078	18.3256	3.14573

APPENDIX B

Liquid Cell Spectra for All Fuels
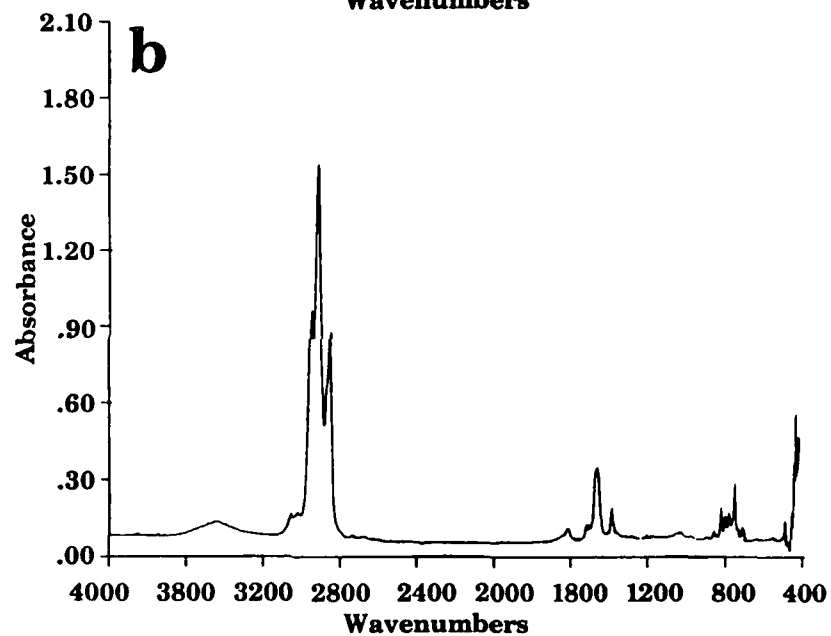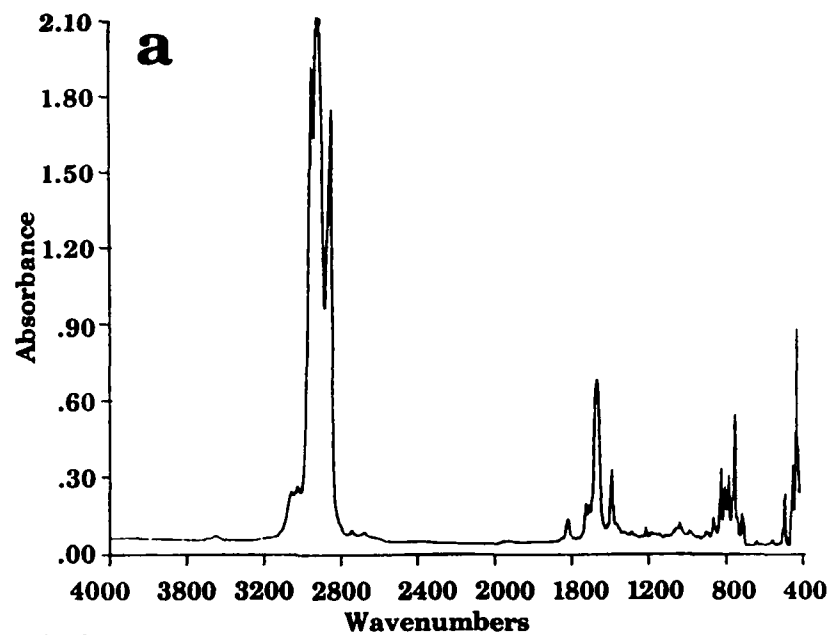
Figure B-1. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel UTRC-2A.
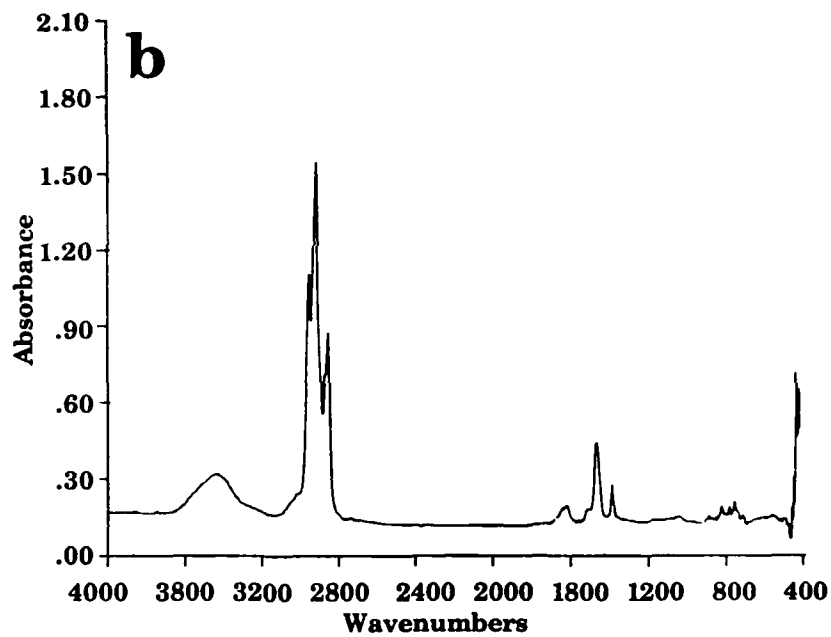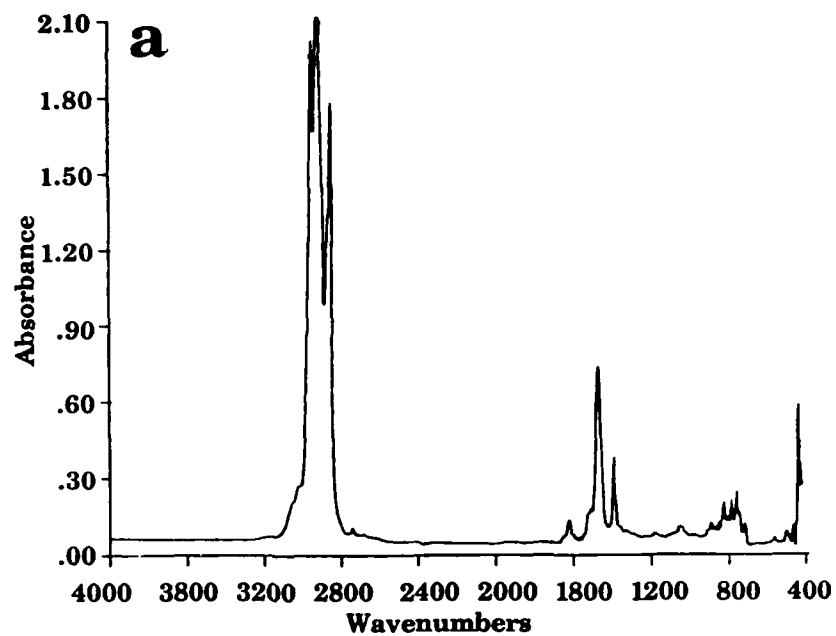
Figure B-2. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel ERBLS-1.
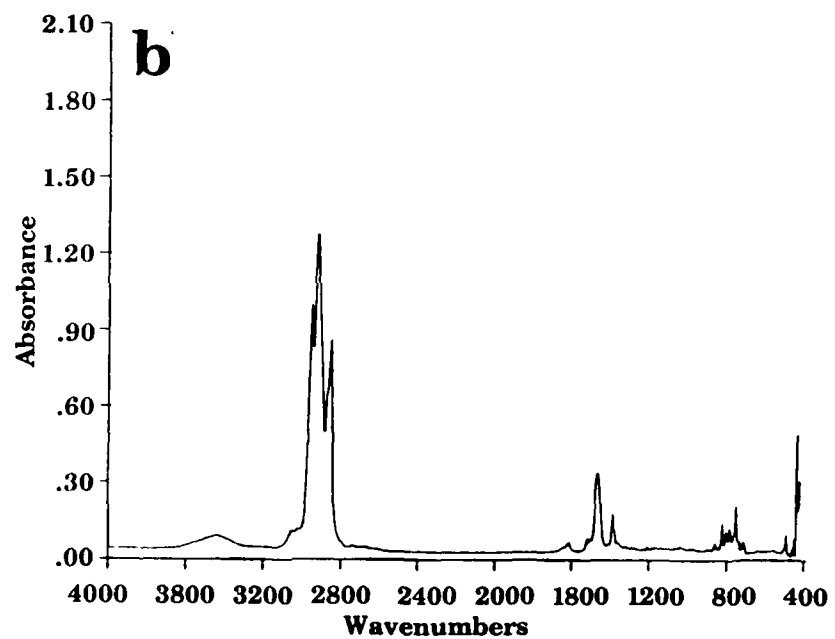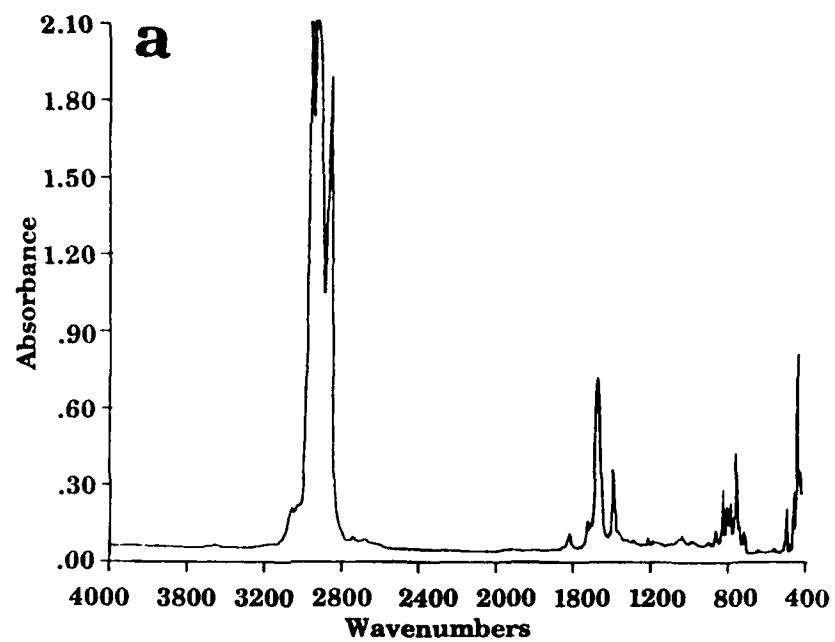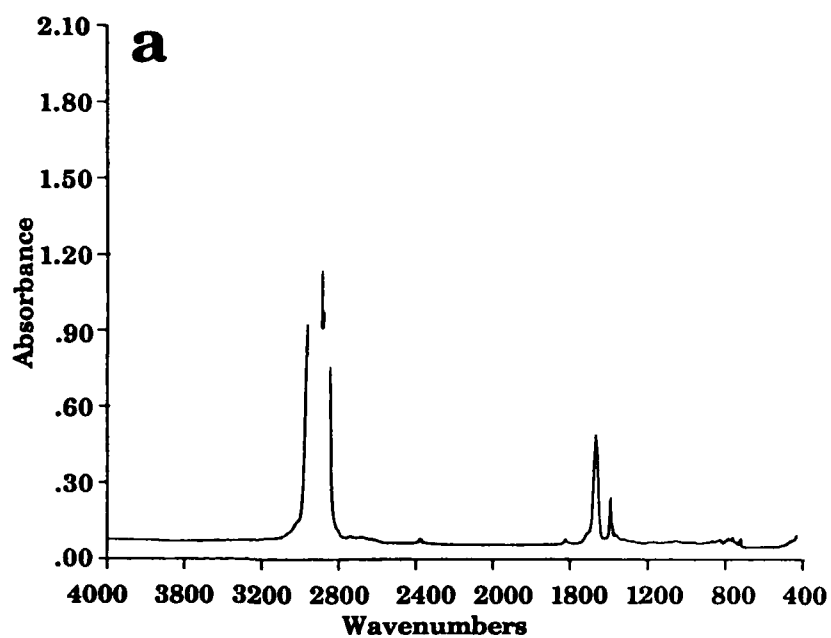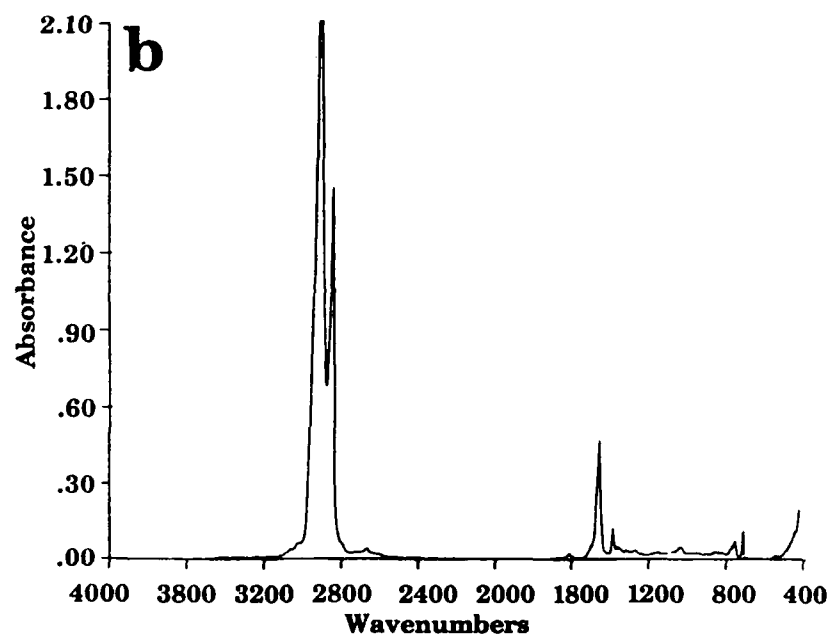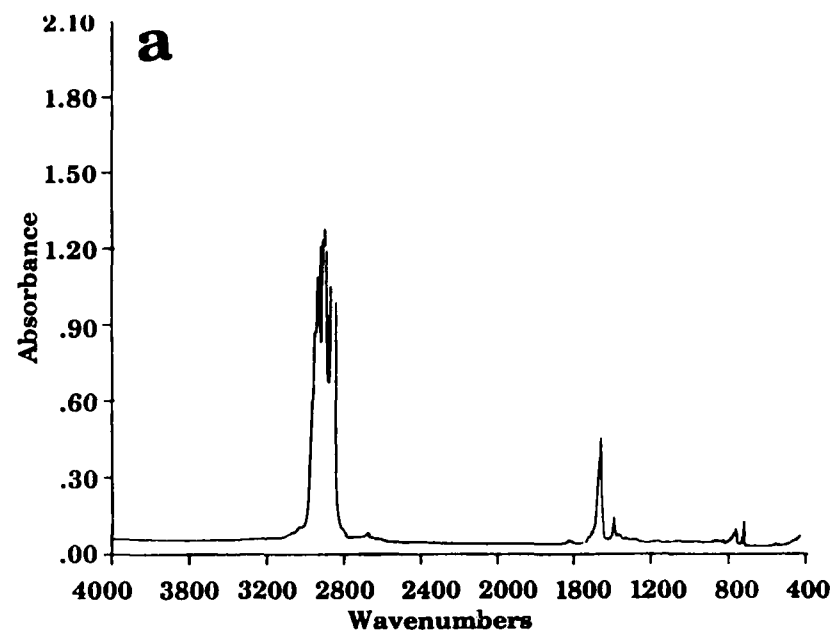
Figure B-3. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel UTRC-7A.
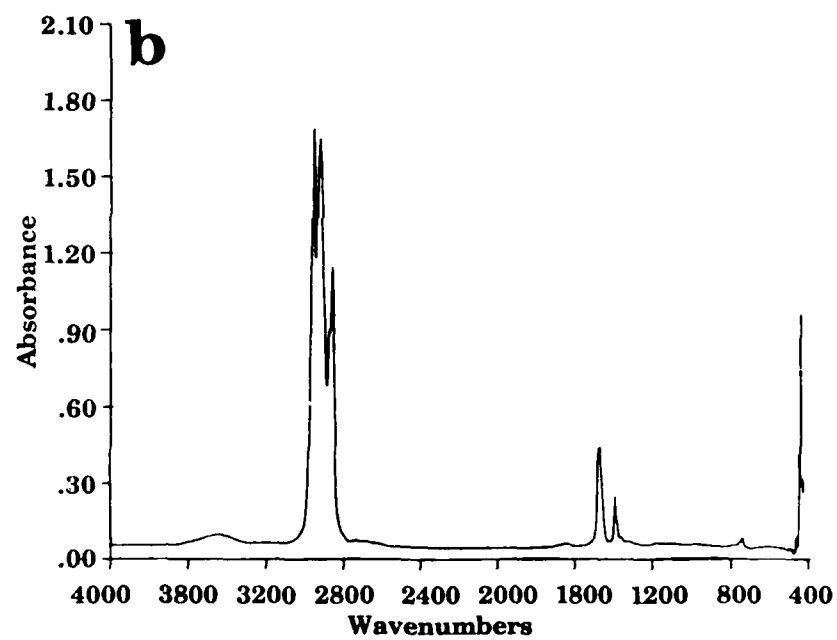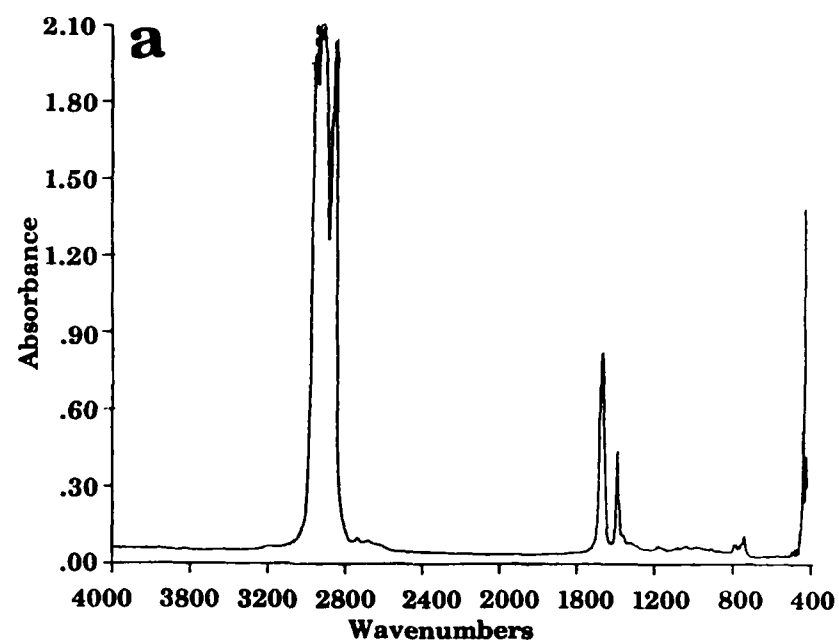
Figure B-4. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel JP-7.
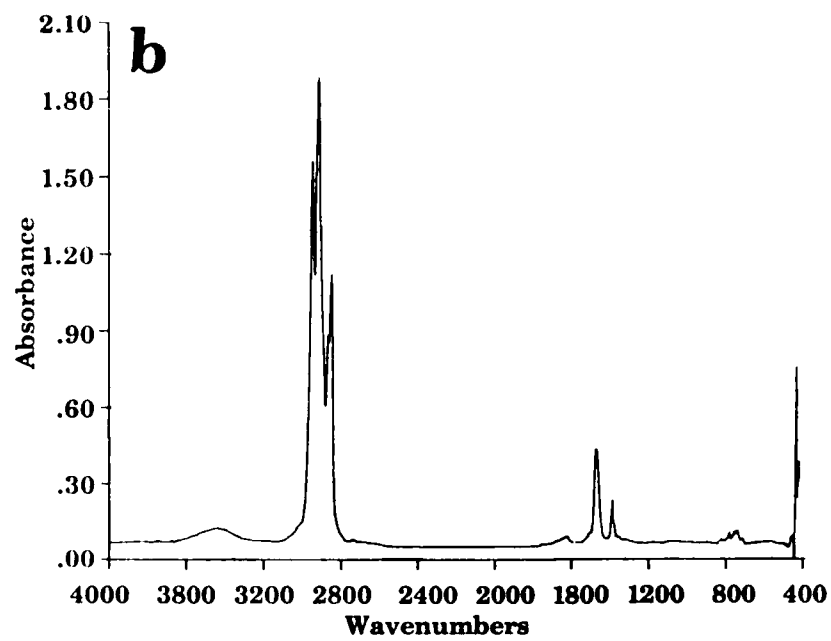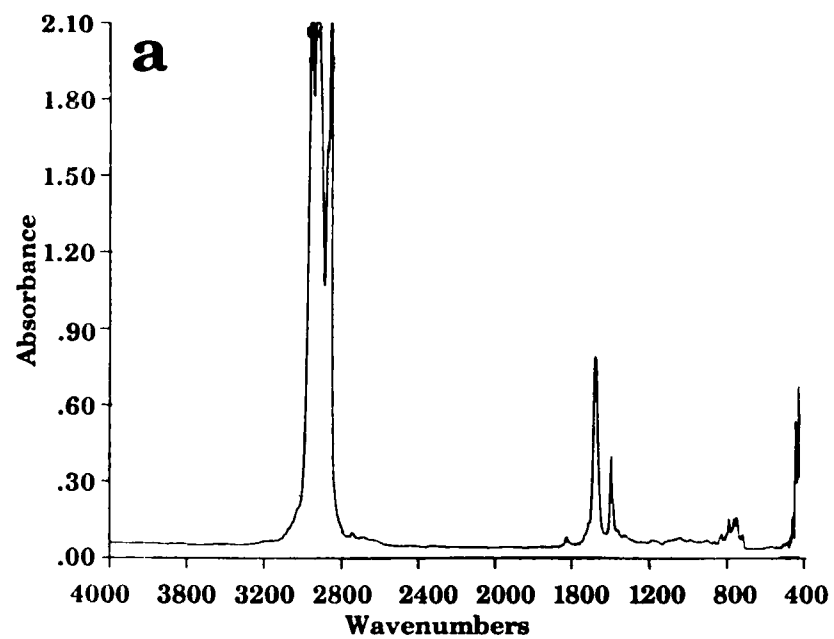
Figure B-5. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel JP4-S.
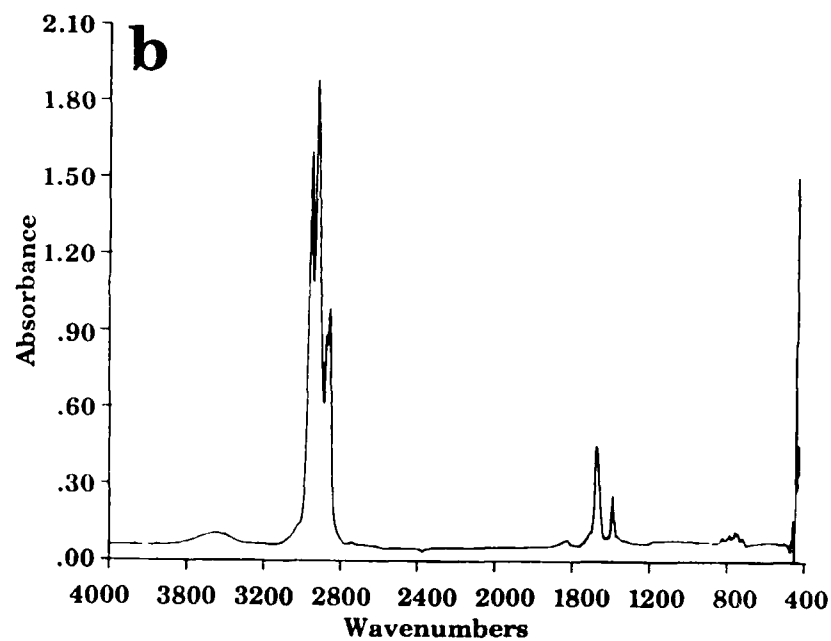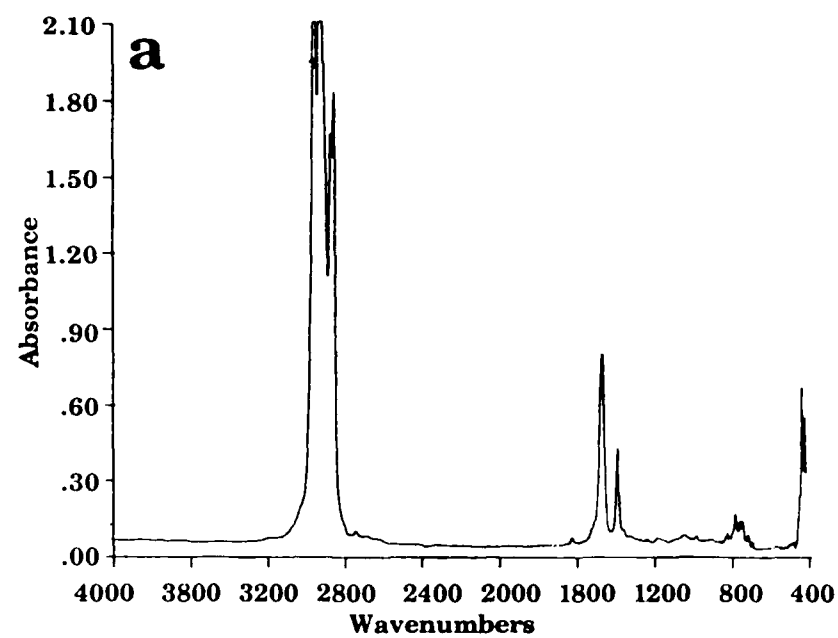
Figure B-6. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel JP4.
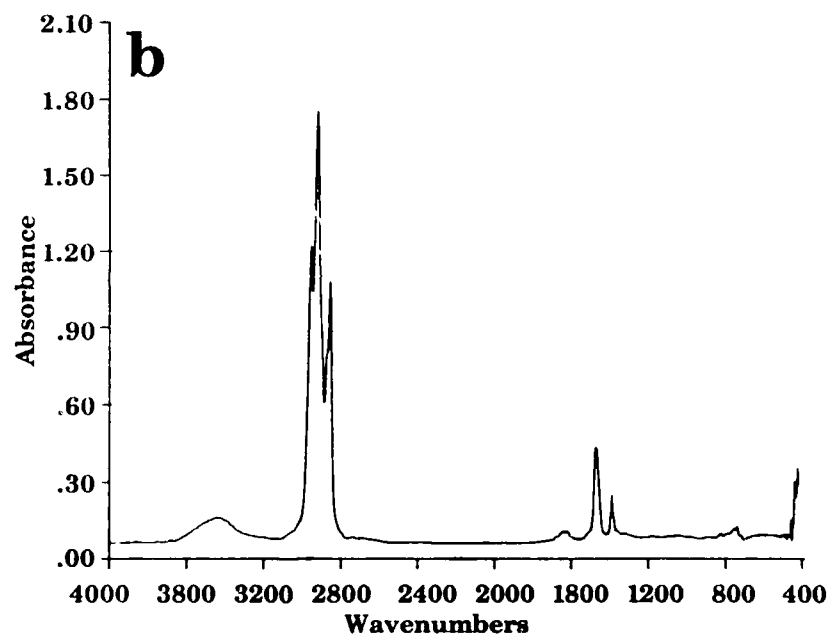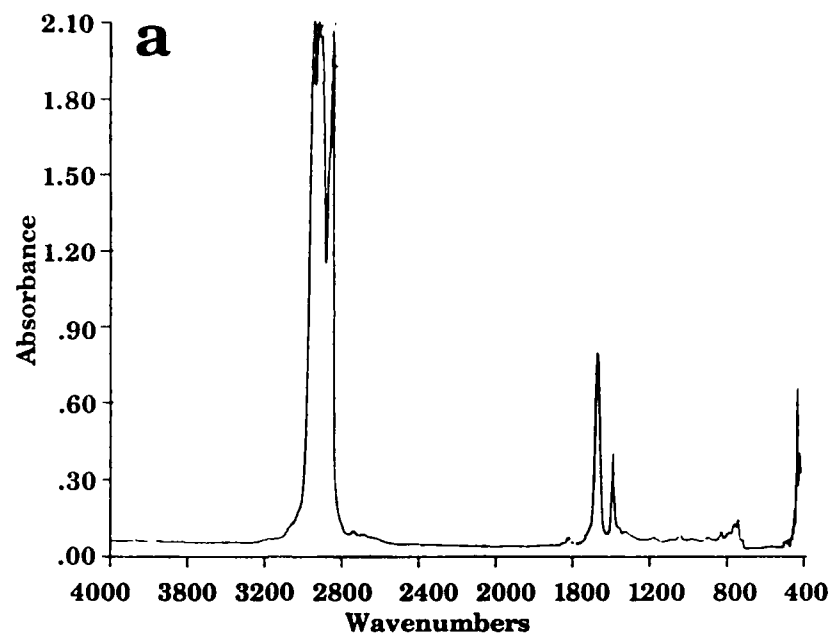
Figure B-7. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel DF-2.
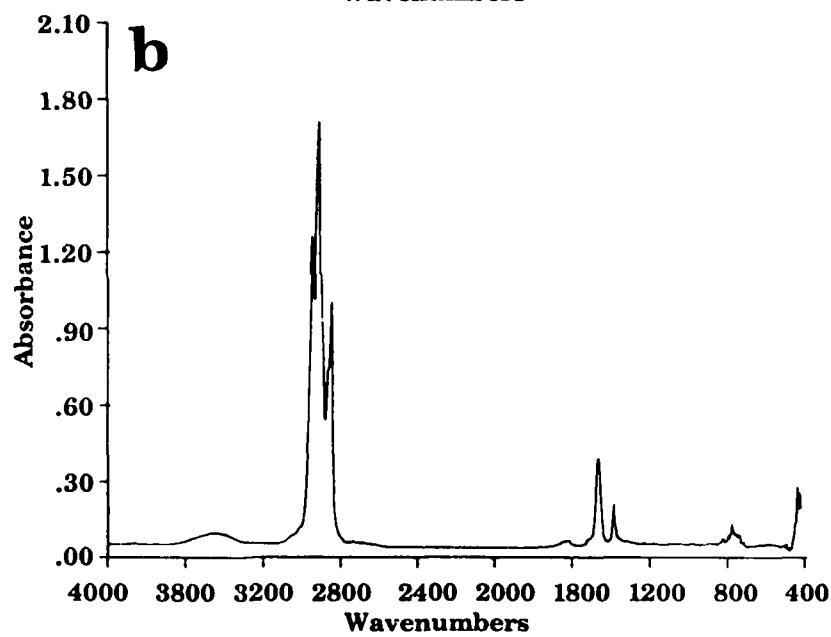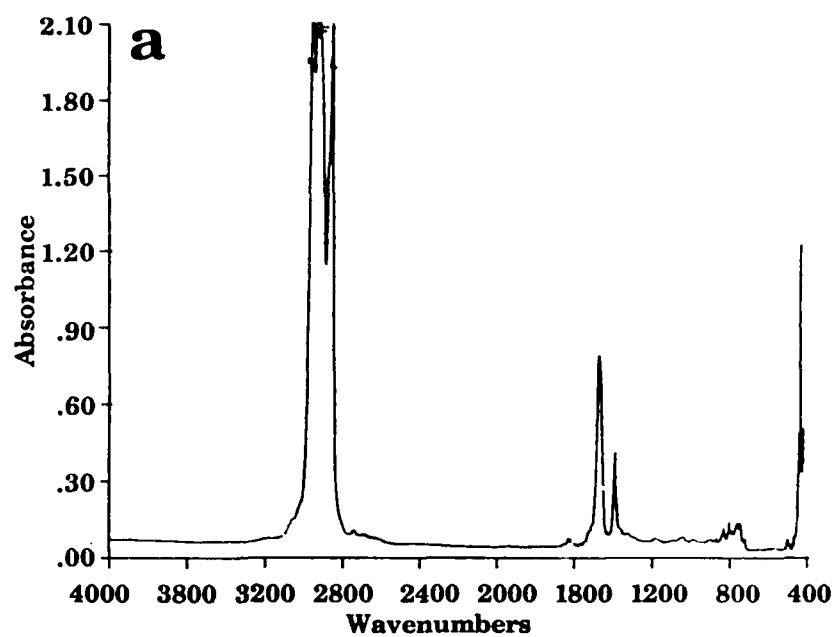
Figure B-8. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel AFAPL-6.
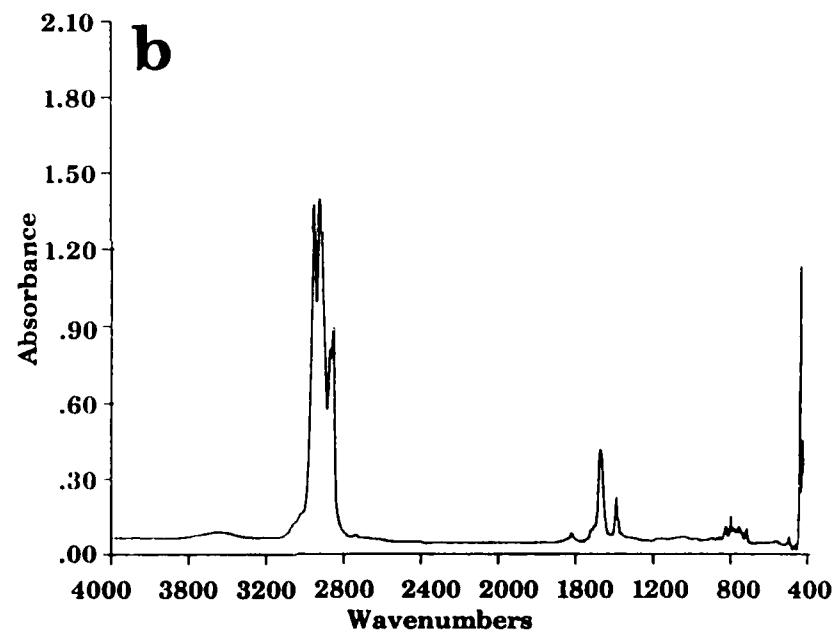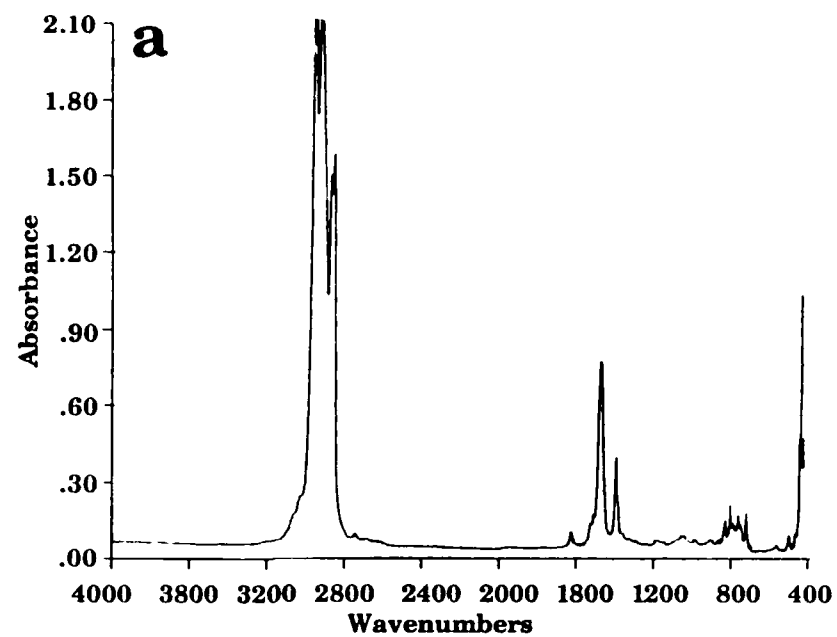
Figure B-9. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel AFAPL-2.
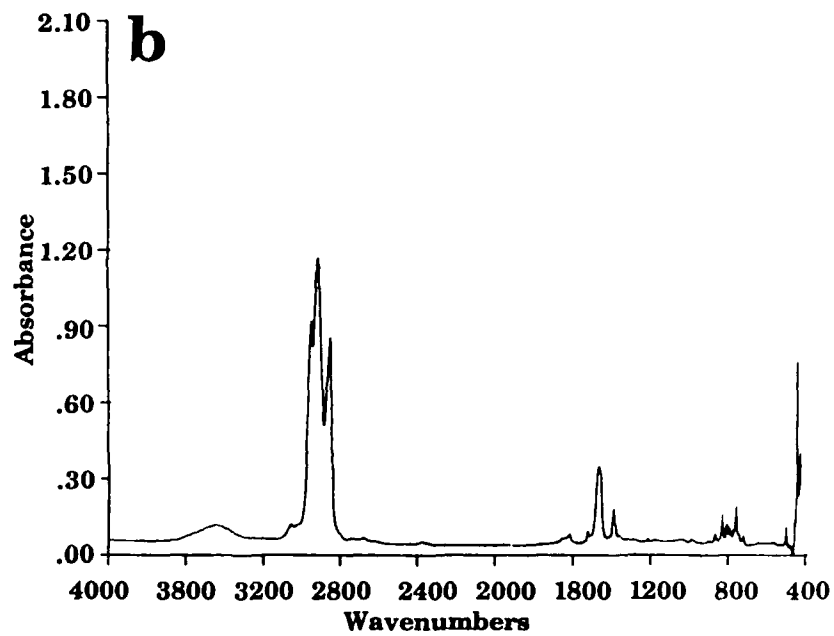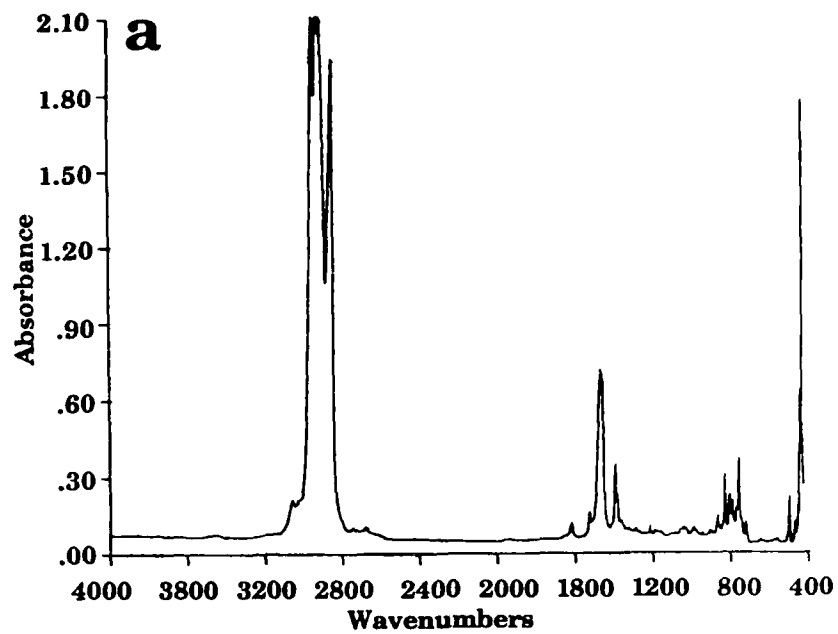
Figure B-10. a) Fixed Path Length Cell and b) Scaled Variable Path
Length Cell for Fuel UTRC-3B.
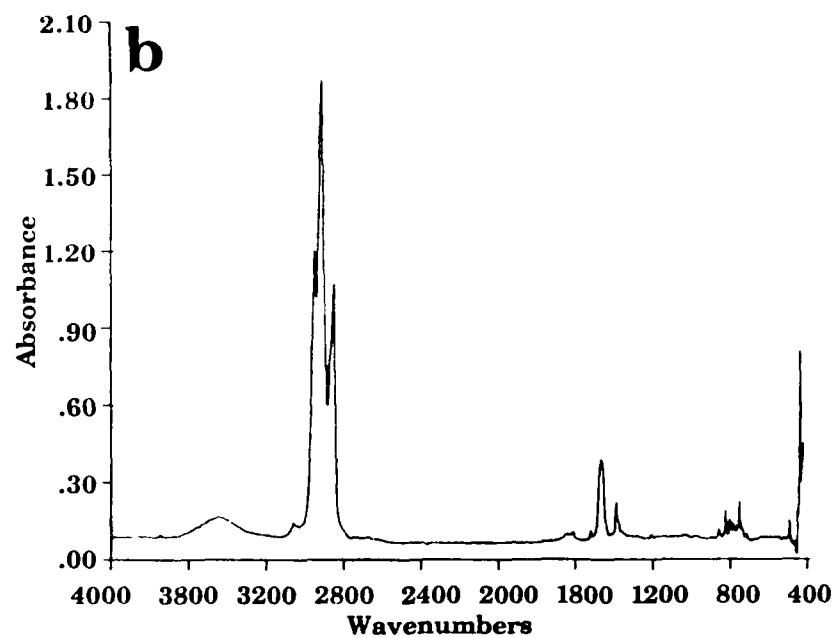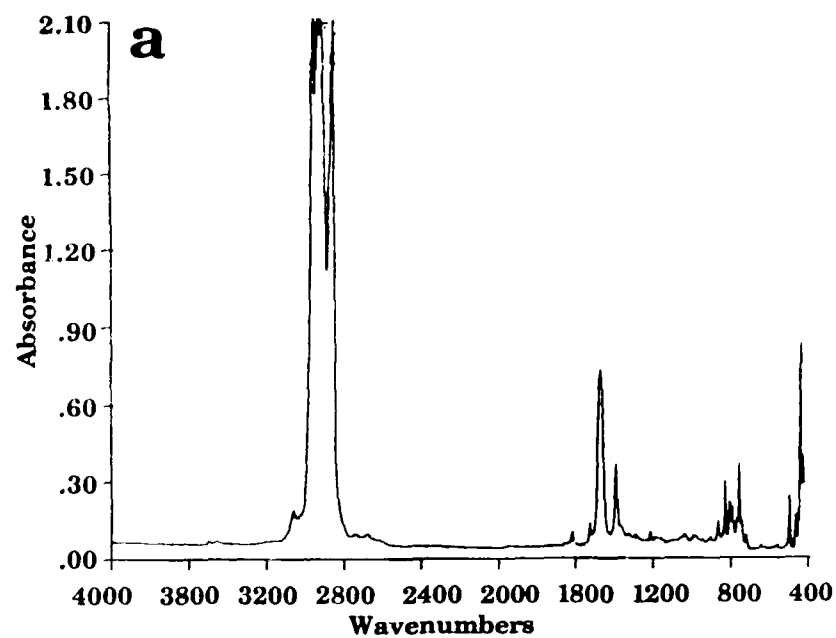
Figure B-11. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel UTRC-8A.
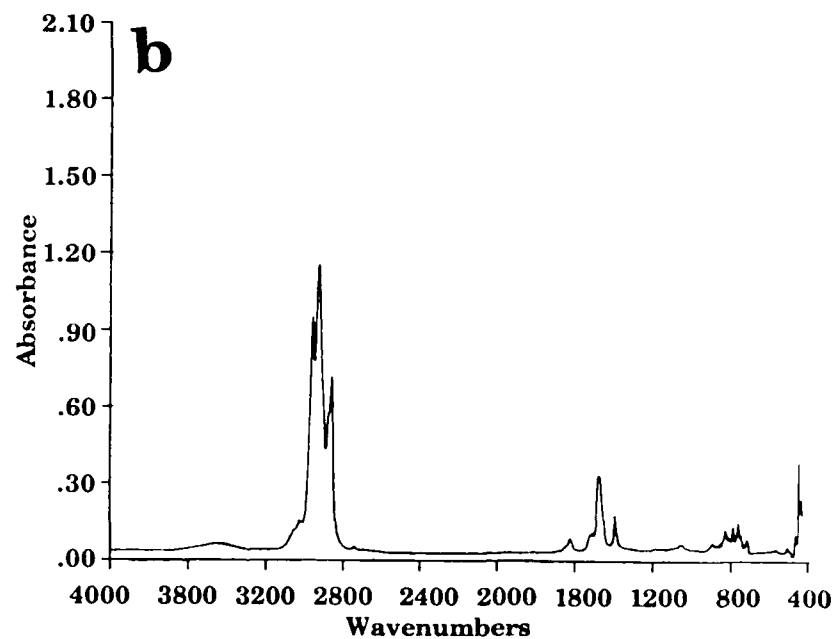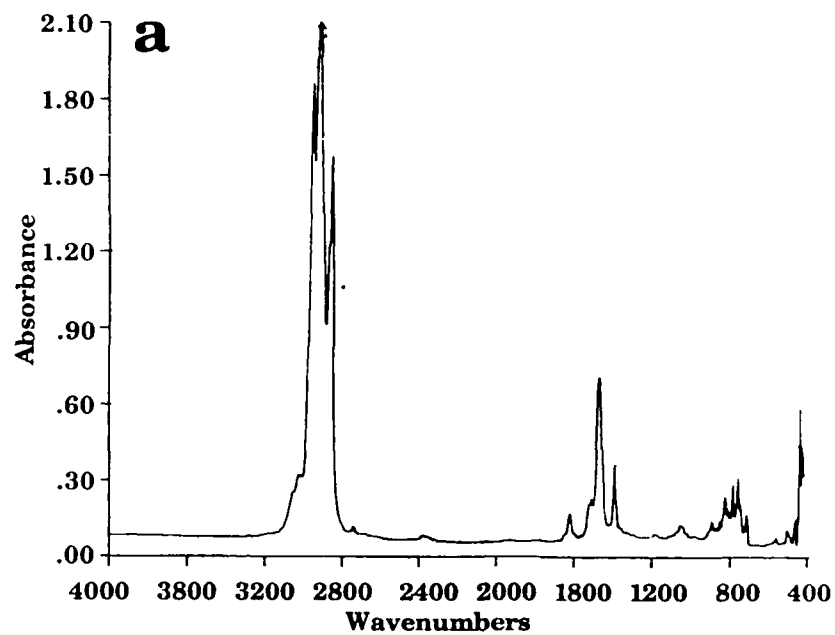
Figure B-12. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel ERBLS-2.
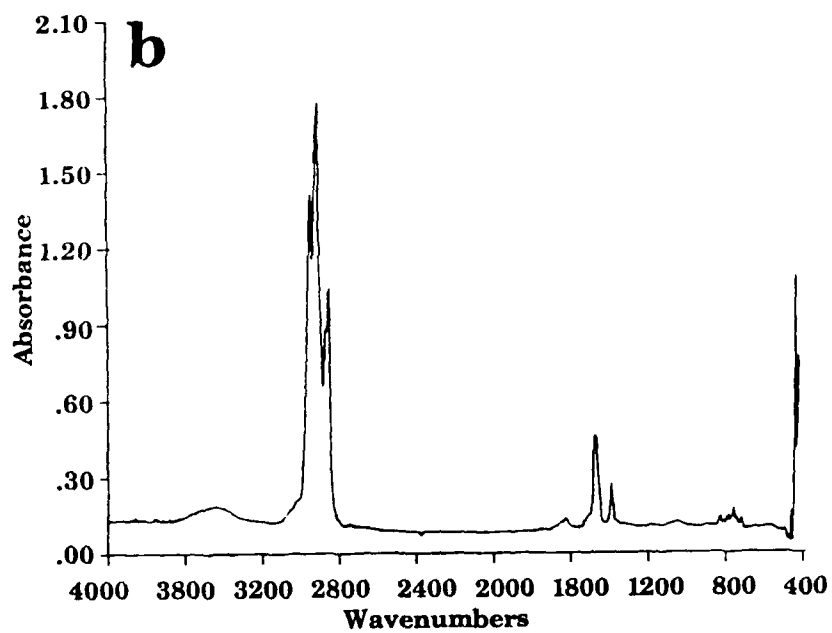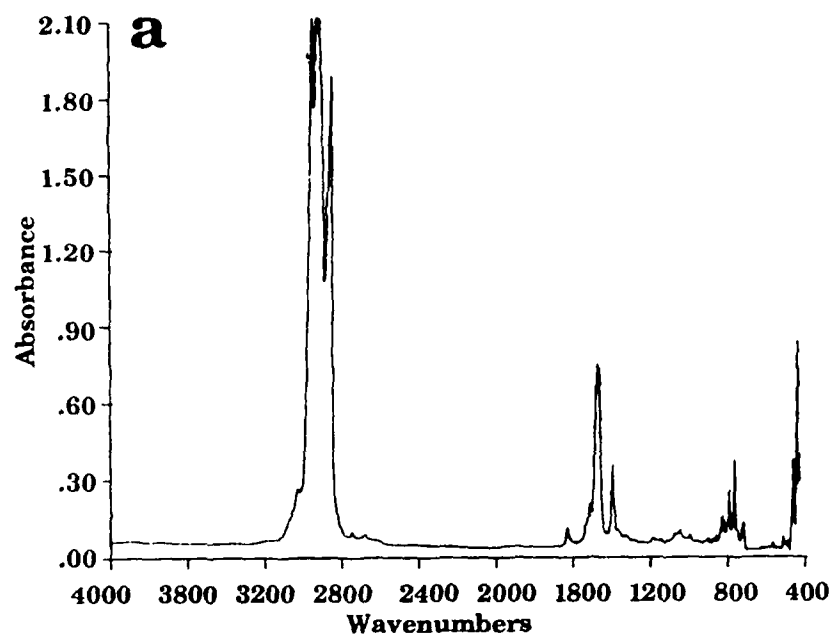
Figure B-13. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel UTRC-9A.
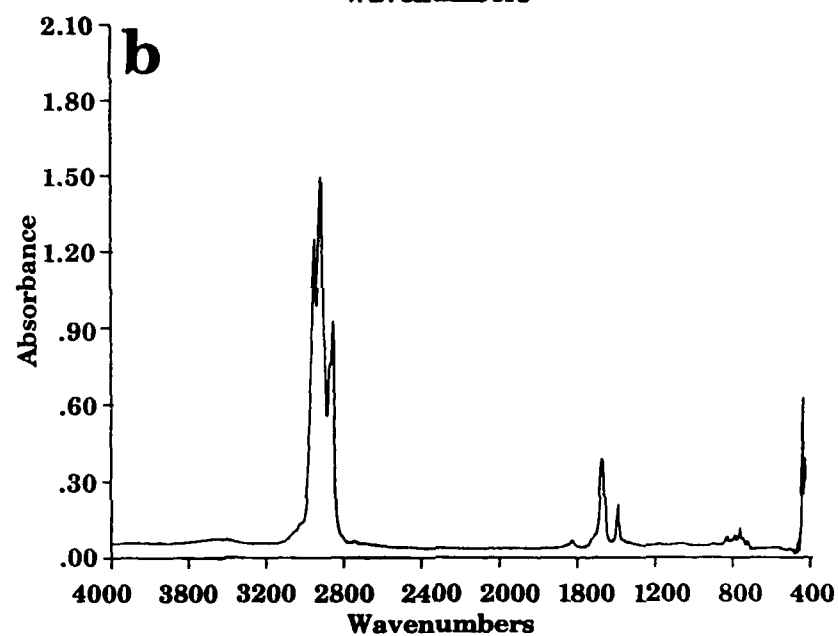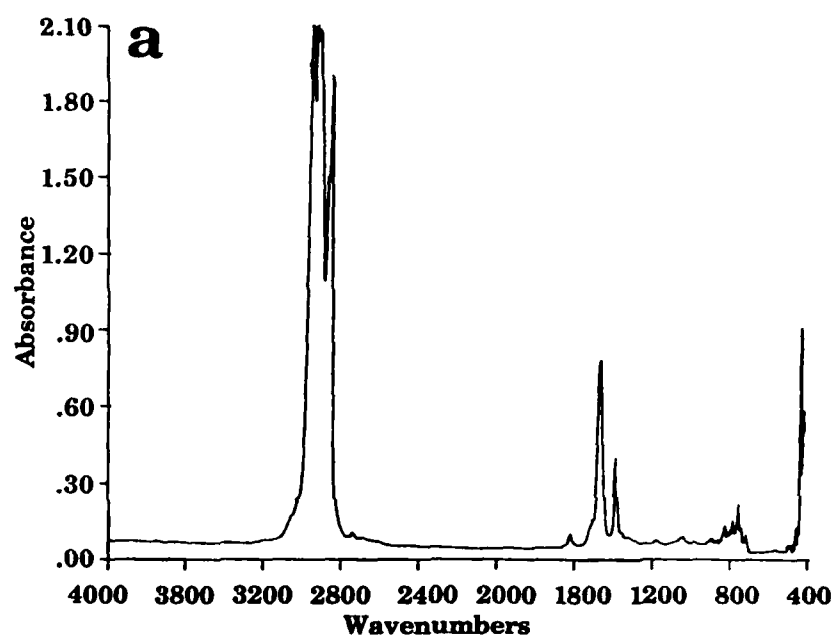
Figure B-14. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel UTRC-9B.
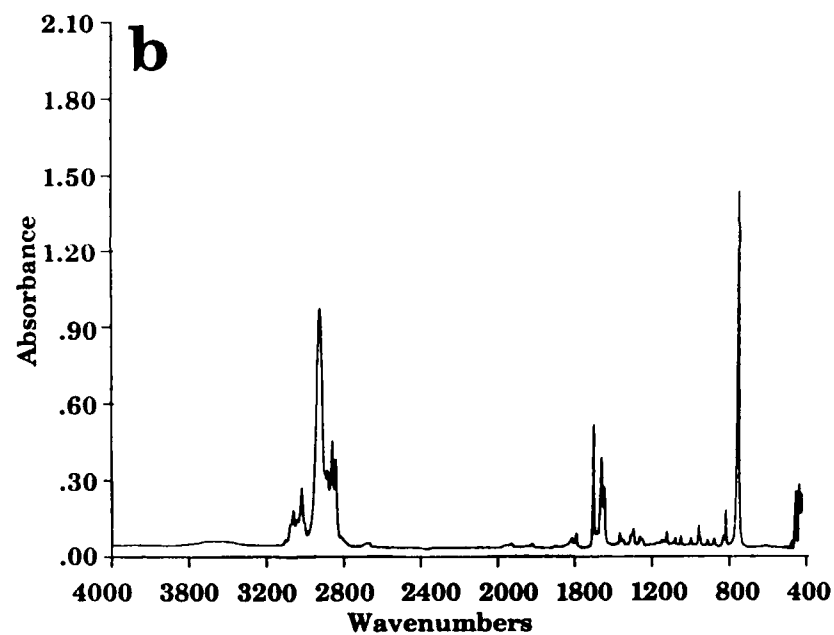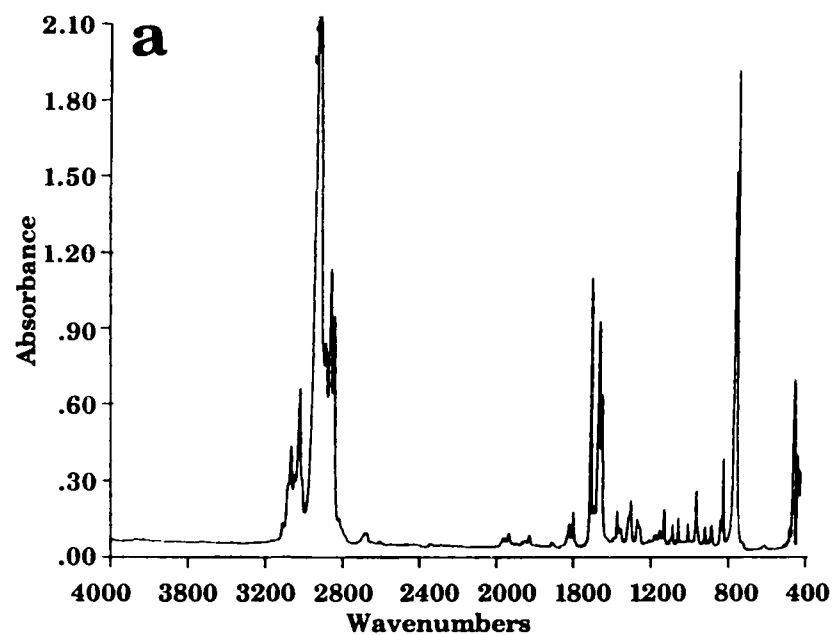
Figure B-15. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel Tetralin.
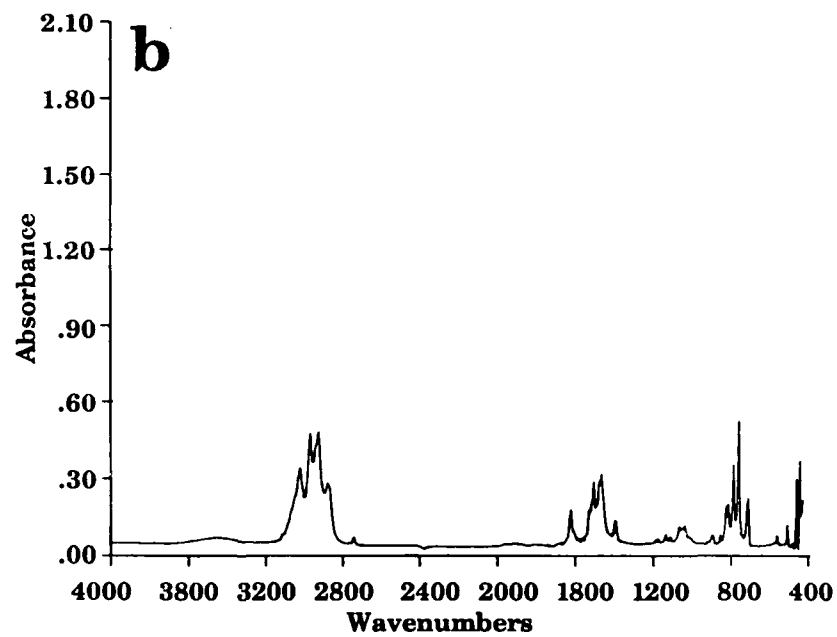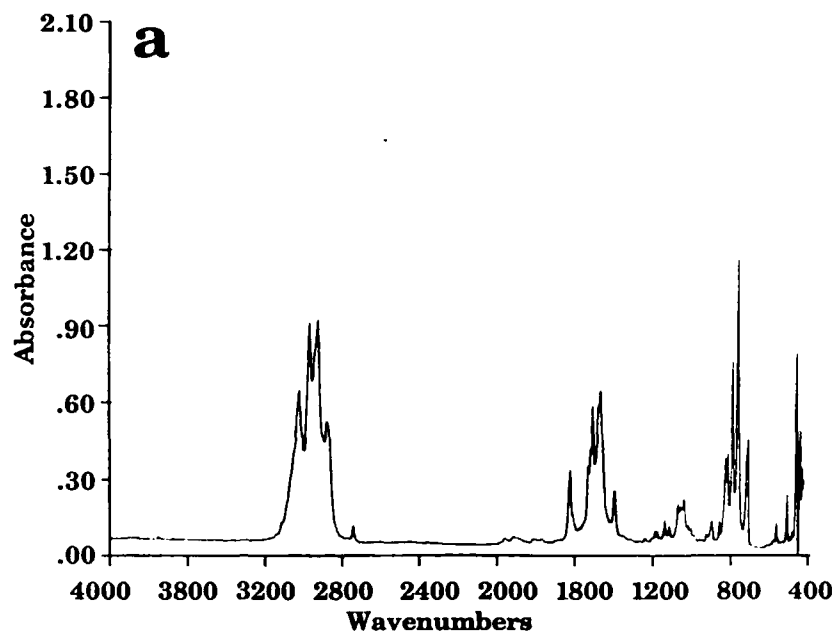
Figure B-16. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel XTB.
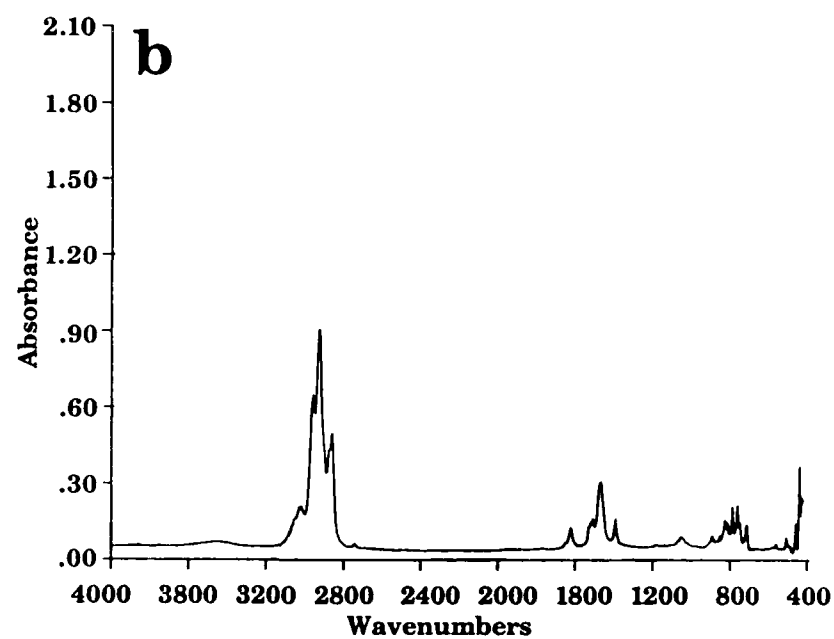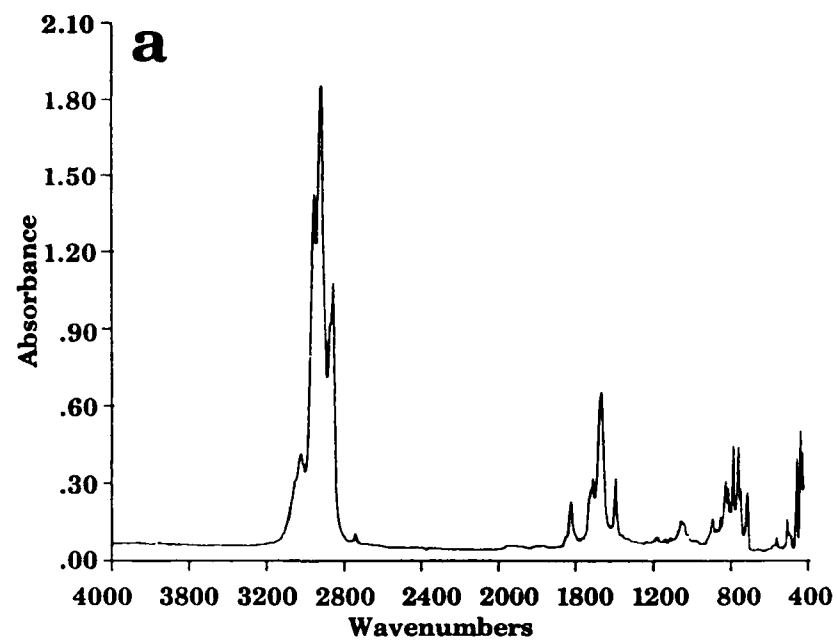
Figure B-17. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel BLS.
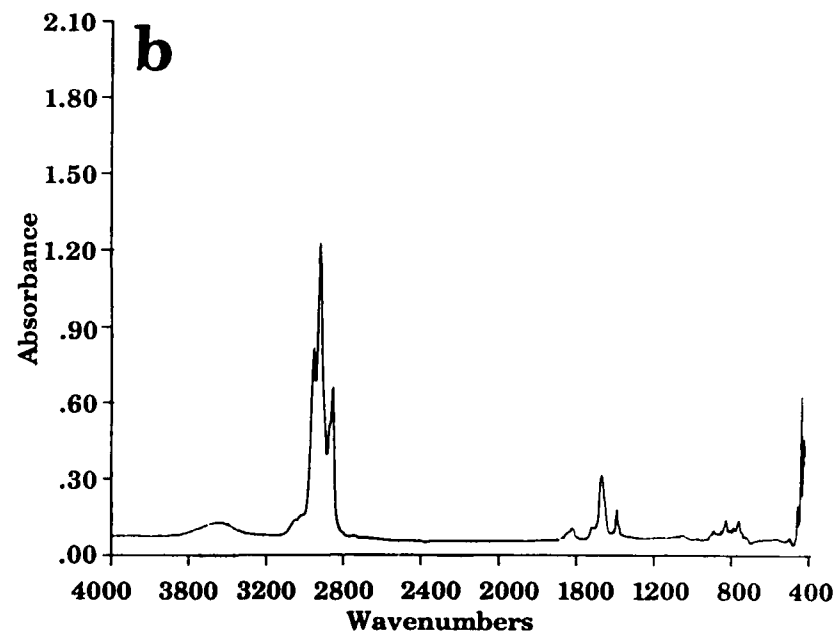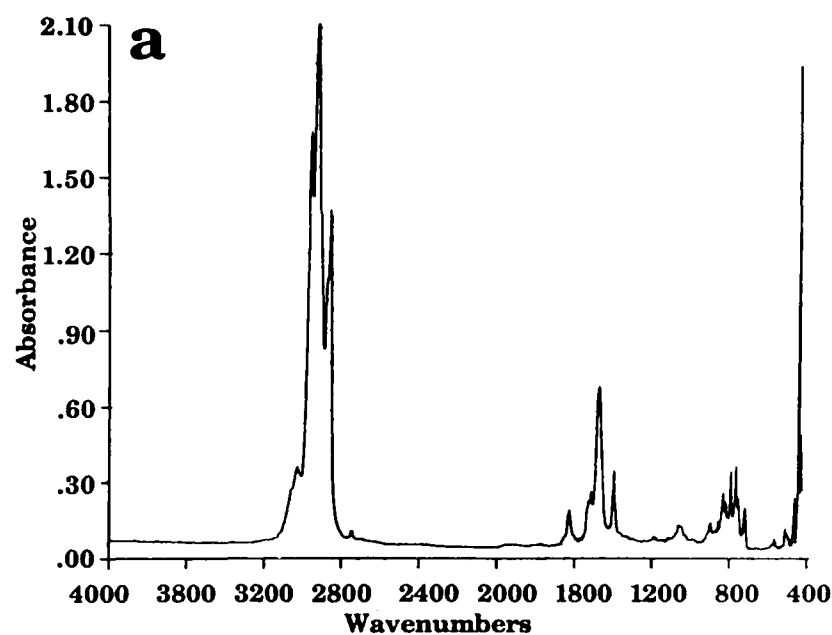
Figure B-18. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel ERBLS-3.
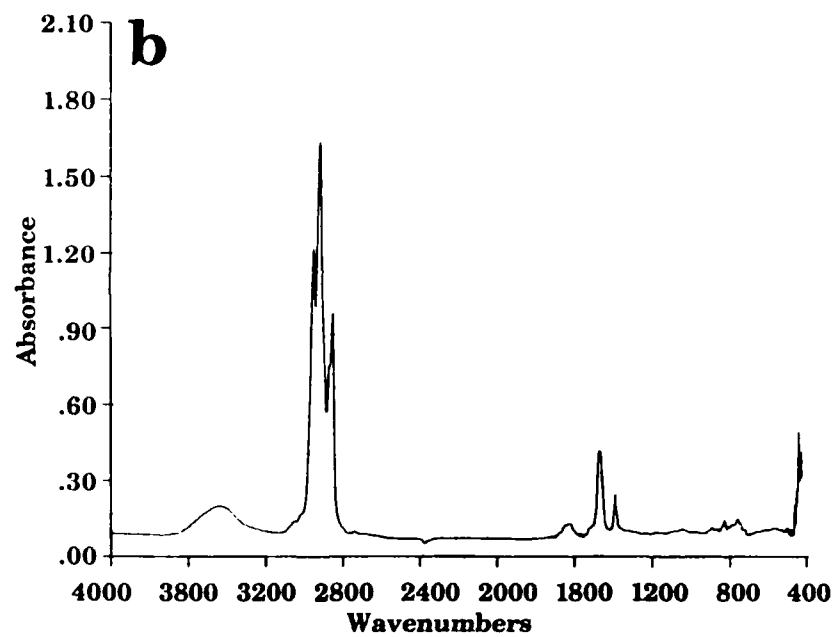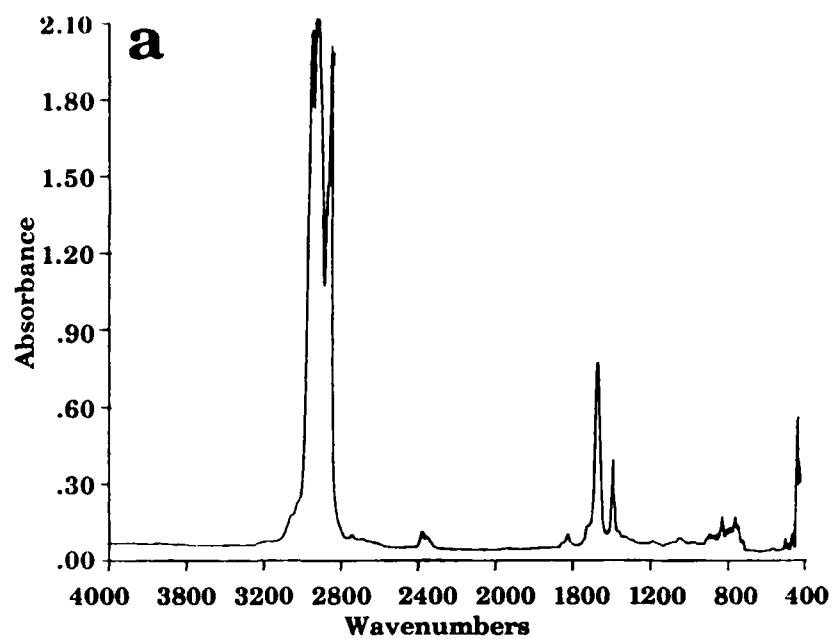
Figure B-19. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel ERBS.
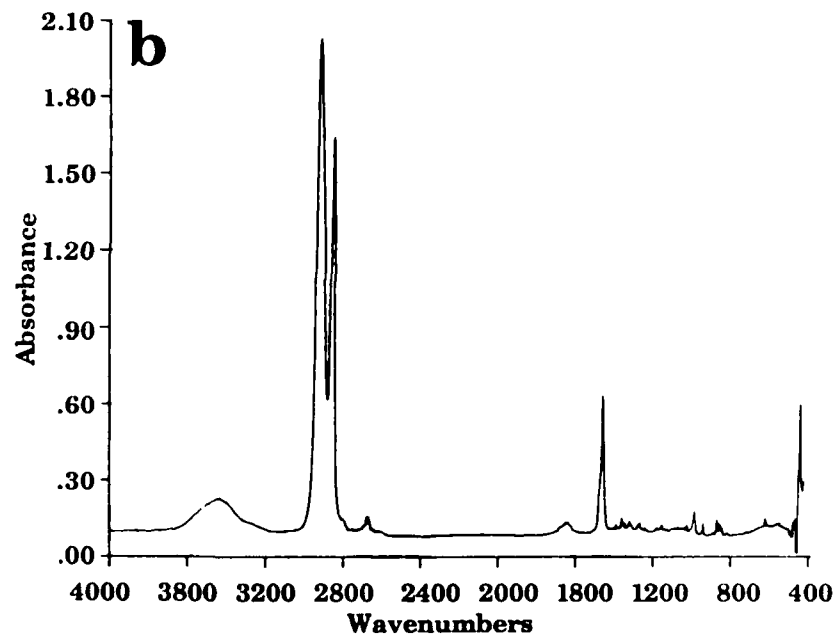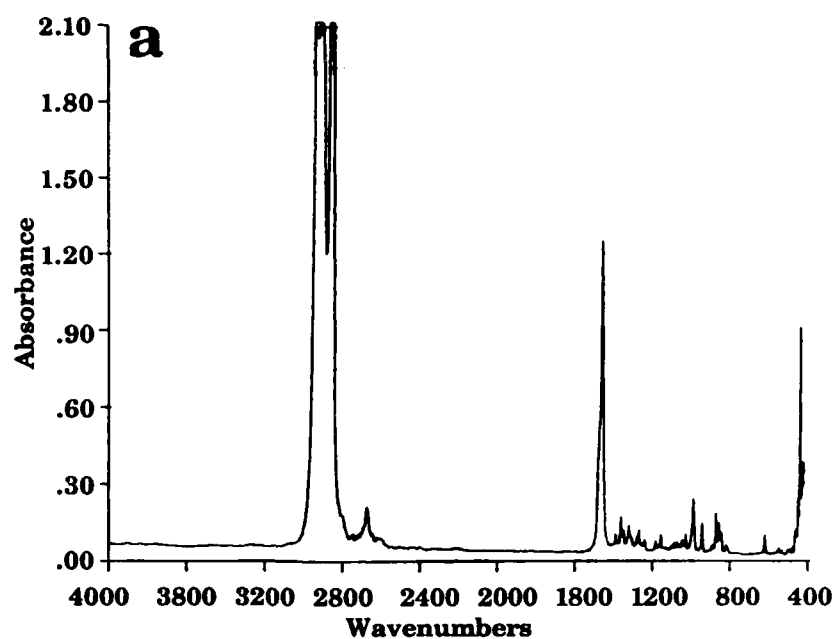
Figure B-20. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel Decalin.
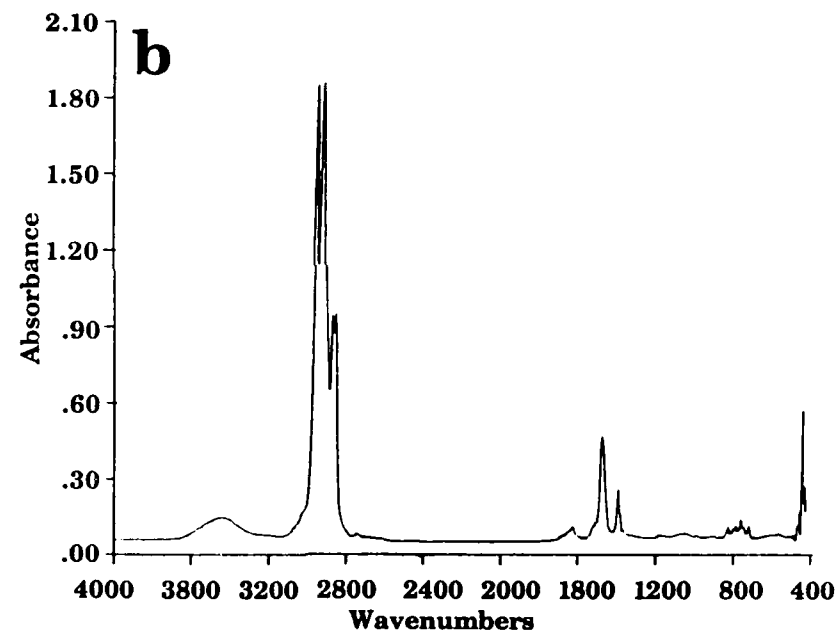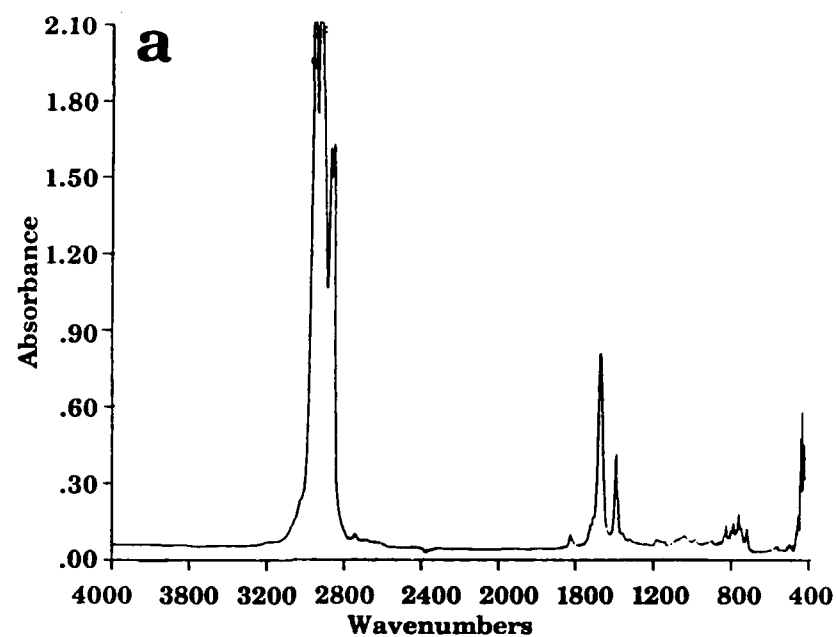
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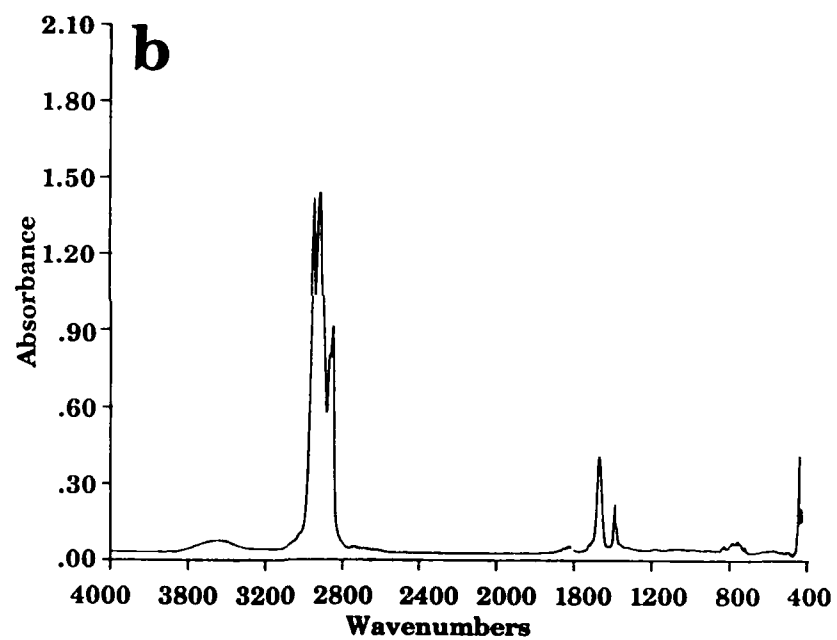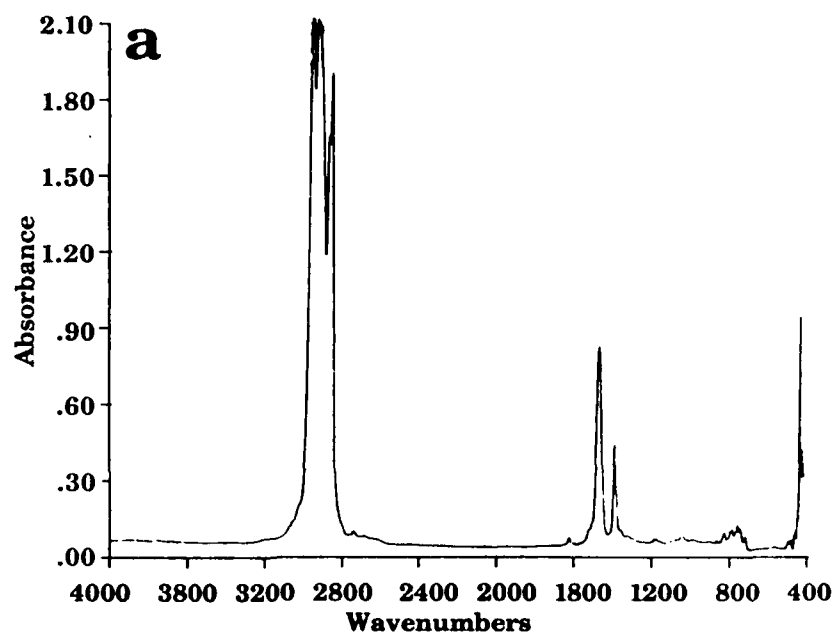
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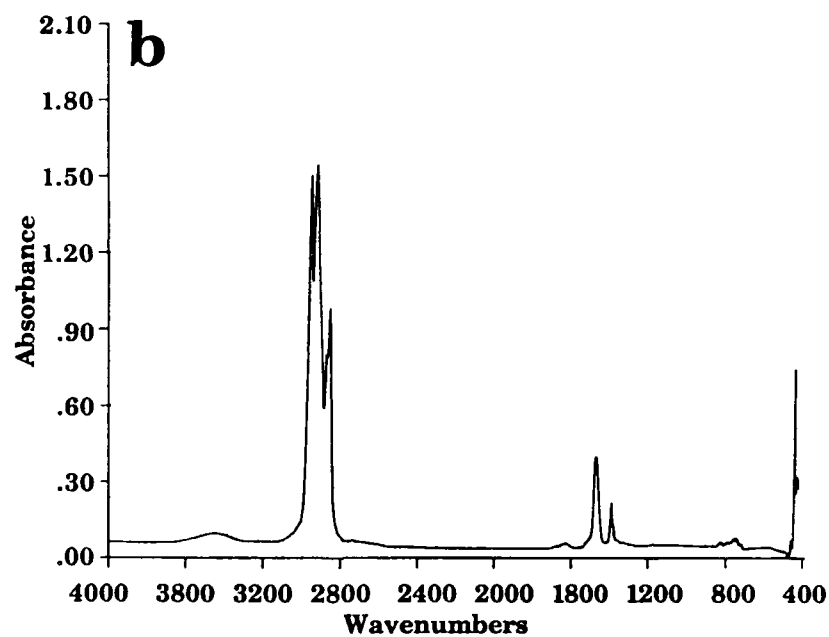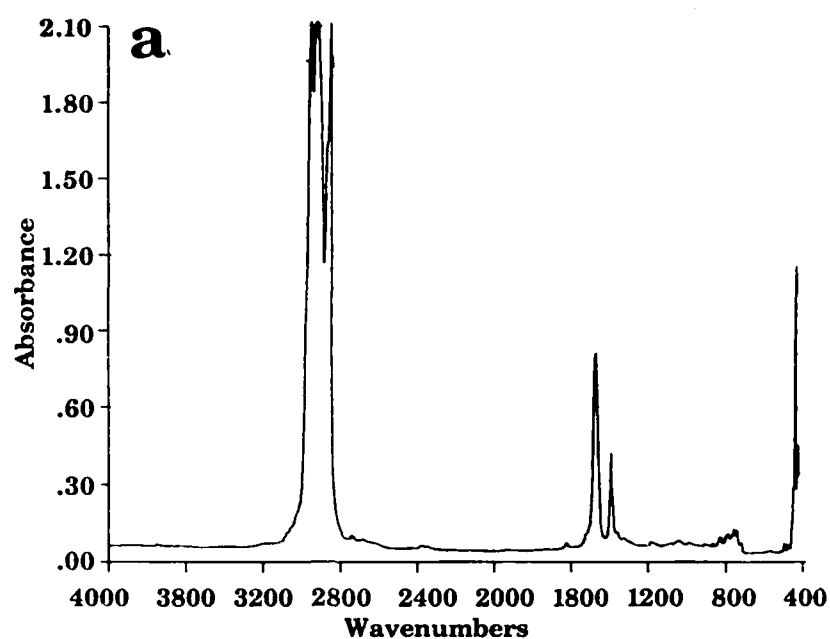
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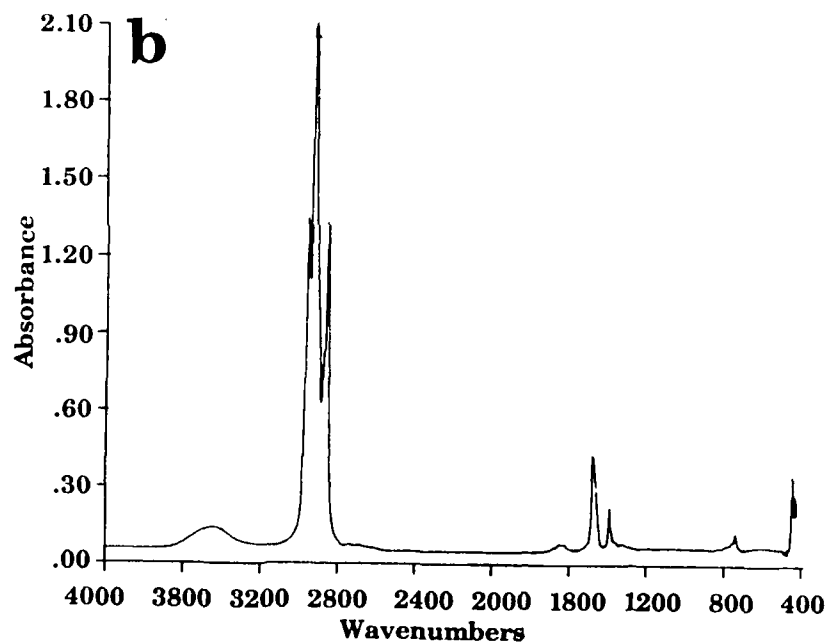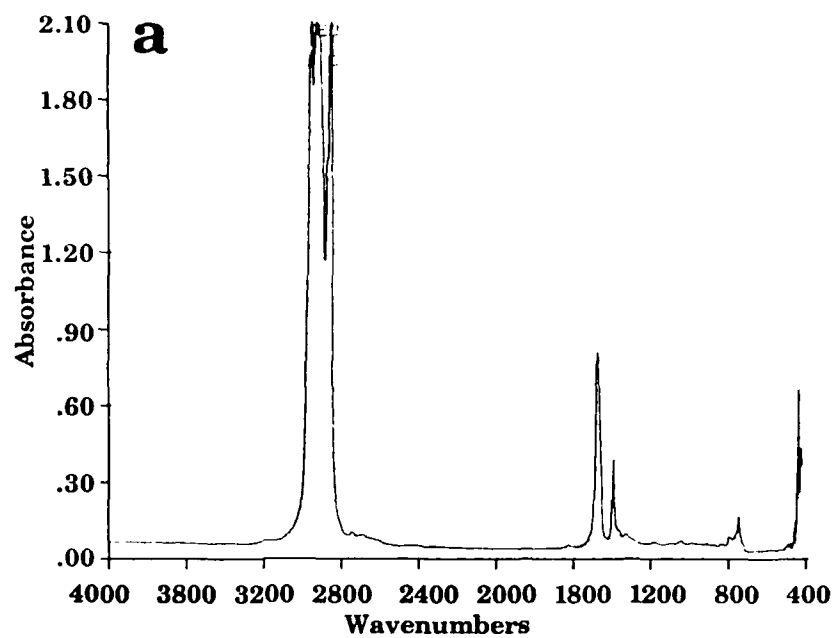
Figure B-24. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel GMSO.
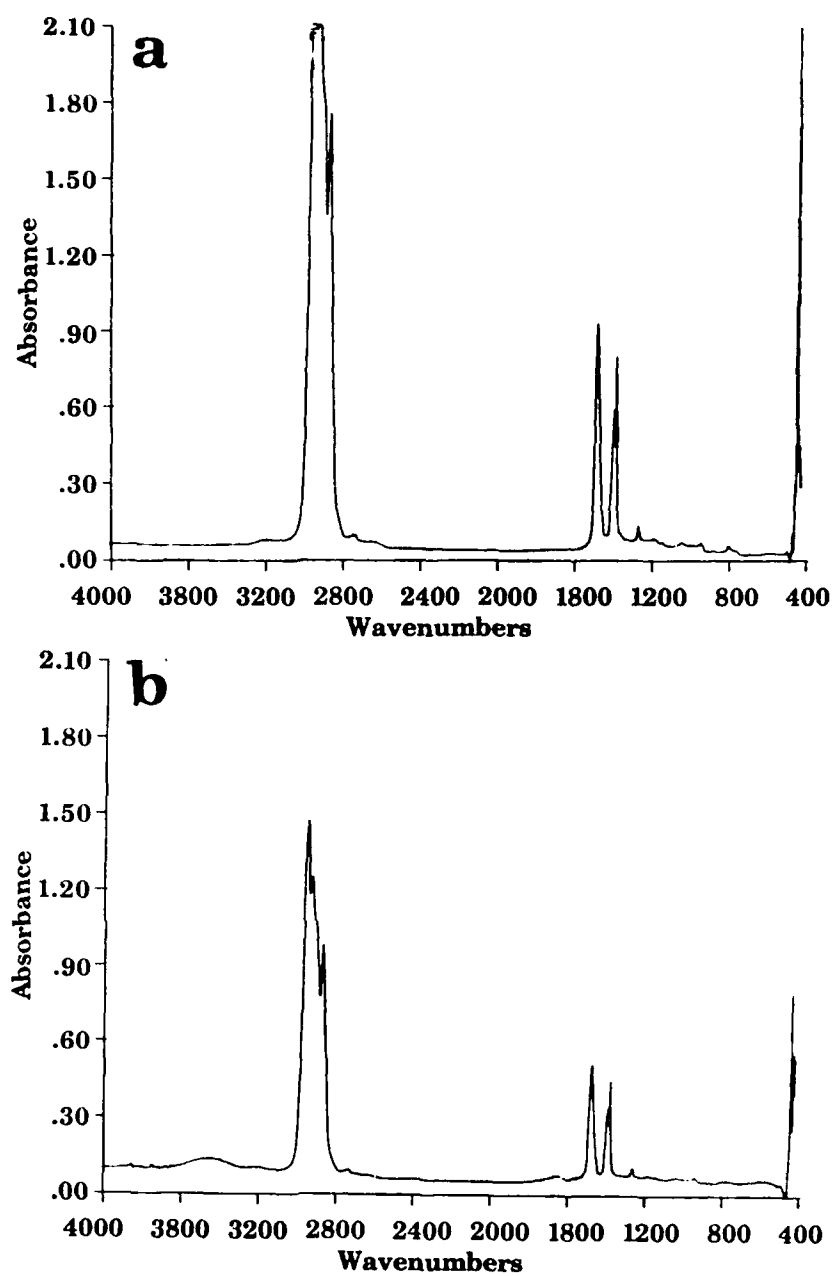
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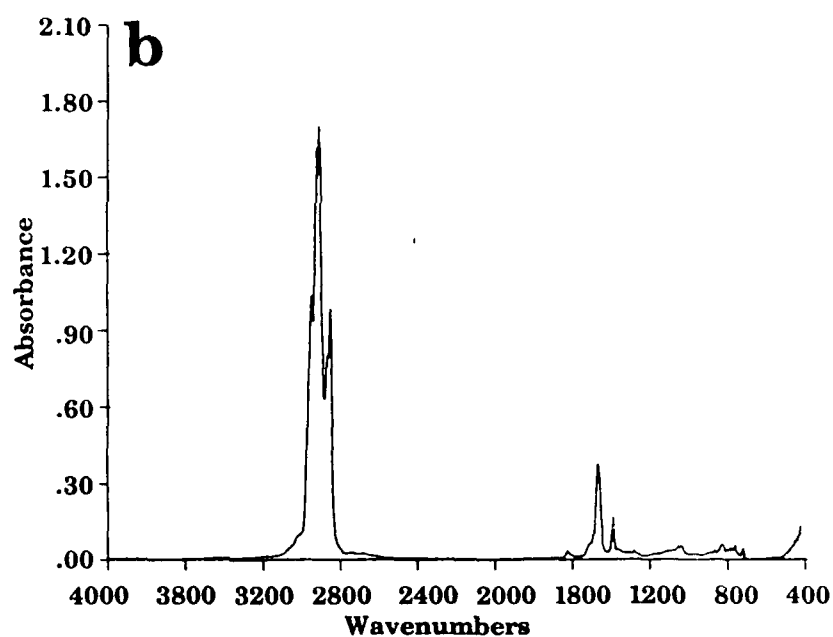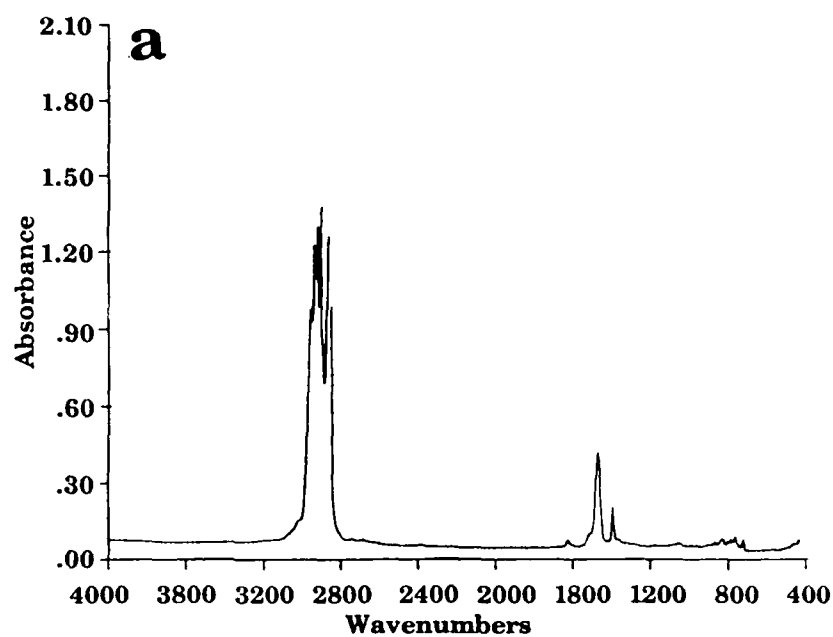
Figure B-26. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel JP8X-2414.
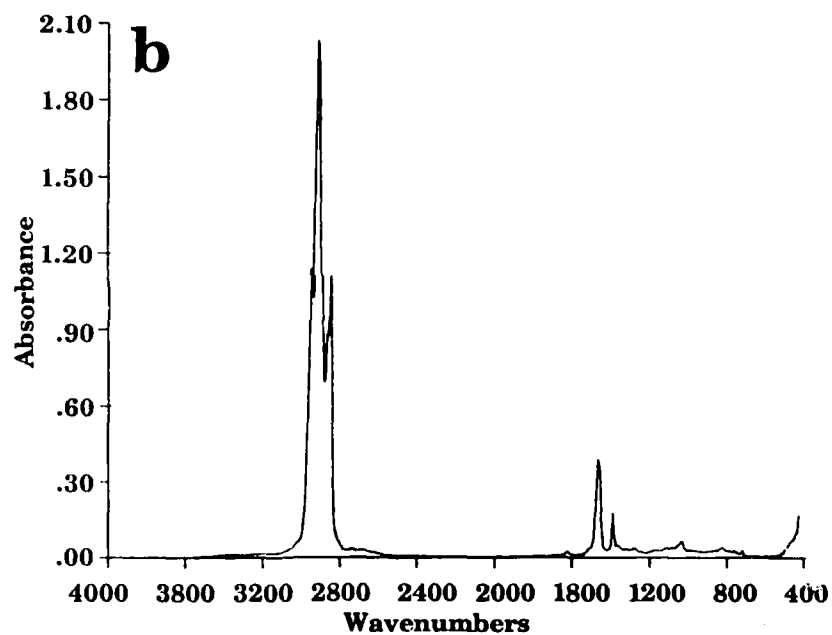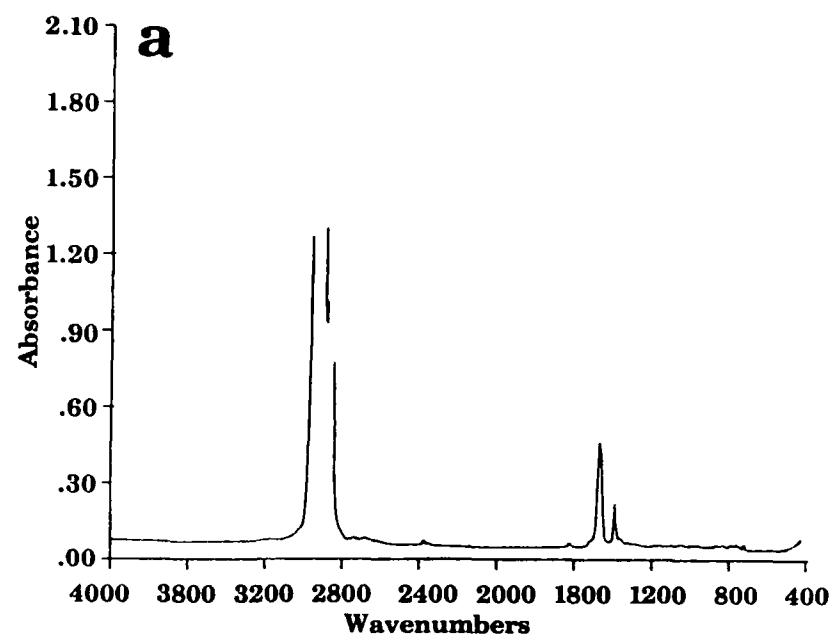
Figure B-27. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel JP8X-2383.
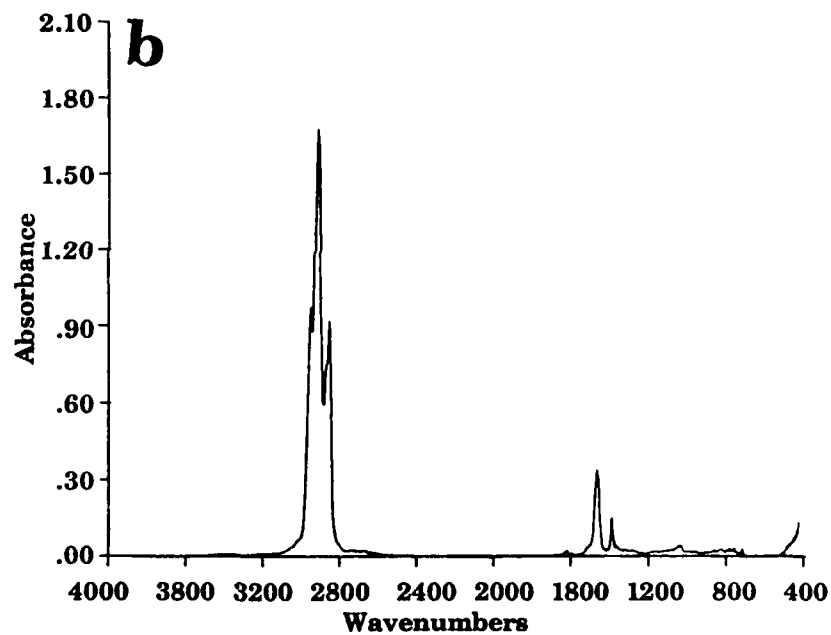
Figure B-28. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel JP8X-2398.

Figure B-29. a) Fixed Path Length Cell and b) Scaled Variable Path Length Cell for Fuel JP8X-2429.

APPENDIX C

A Kinetic Model for the Pyrolysis of Large n-Alkanes

A KINETIC MODEL FOR THE PYROLYSIS OF LARGE n-ALKANES

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ABSTRACT

A new kinetic model describing the pyrolysis of complex mixtures of n-alkane hydrocarbons is presented. This free radical model is based on conventional elementary reaction steps and rate constants from the literature. In developing this model, we have extended the basic Rice, Kossiakoff, and Herzfeld (RKH) mechanism to higher temperatures by adding more decomposition, addition and hydrogen-transfer reactions. A further modification of RKH was to drop the assumption that heavy radicals always isomerize before decomposition. Isomerization rate constants were included to determine the extent of isomerization in competition with the other processes which can create or destroy large radicals. A solution procedure was developed involving three simplifying assumptions: 1) steady state radical populations, 2) single termination rate for all radicals, 3) use of stoichiometric coefficients to describe the distribution of radicals over various carbon numbers in large n-alkyl and n-alkenyl radicals. Extensive simulations were made of literature and in-house data to test the model predictions and assumptions. Results are presented for simulation of flow reactor data for butane (1373 K, 1 atm), hexadecane (866-977 K, 65 atm.), and Solpar (a C_{12}-C_{18} mixture, 1053 K, 1 atm.) pyrolysis and of shock tube data for octane pyrolysis and hydropyrolysis (1000-1500 K). In general, the model provides good predictions of product distributions and the overall cracking rate up to 1400 K. At temperatures above 1000 K the overall rate is somewhat overpredicted. At temperatures above 1300 K and high extents of reactions, the predictions for major species deviate somewhat from the data. Possible reasons for these discrepancies are given, and include the lack of treatment of secondary pyrolysis of olefins and diolefins and possible errors in the initiation rates at high temperatures.

Topics: Kinetics; Thermal Decomposition; Soot

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INTRODUCTION

Soot production in combustion is an important phenomenon which can influence heat transfer rates, flame stabilities, reaction temperatures, conversion efficiencies, pollutant release rates, and the life expectancy of combustion devices. Glassman has shown that the tendency to form soot during combustion increases as alkane chain lengths increase (1). These heavy alkanes are major components of kerosenes and gas oils and are thought to be important generators of soot in jet engines and combustors. In order to minimize soot production in these devices, it is, therefore, desirable to develop predictive kinetic models describing the cracking of large alkanes into smaller gases and of these smaller gases into soot. Unfortunately, accurate kinetic models for hydrocarbon cracking have been developed only for hydrocarbons containing less than about five carbons (2).

We have approached the problem of modeling soot formation during the cracking of large alkanes by splitting the model's development into two parts. In the current model the earliest stages of cracking have been described. This initial model provides predictions for the concentrations of H_2, alkanes, 1-alkanes, dienes including acetylene and propadiene, H radical, alkyl radicals, and alkenyl radicals. The computer program can easily be recompiled to handle arbitrarily long hydrocarbon•

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chains, but is presently restricted to straight chain aliphatics. During the second part of our modeling program, we plan to extend this model to include the cracking of olefins and dienes, ring formations via Diels-Alder reactions, and the formation of large polyaromatic hydrocarbons via additions of acetylene to aryl radicals.

MODEL FORMULATION

The cracking of normal alkanes in the temperature range of 400-1000 K is well described by the Rice, Kossiakoff, and Herzfeld (RKH) mechanism (3-7): large alkyl radicals are formed by initiation or hydrogen transfer steps and then decompose via successive β-eliminations of 1-alkanes to make methyl and ethyl radicals. These small radicals then abstract hydrogens from the heavier alkanes to stabilize as methane and ethane and propagate the chain reaction. In the simplest form of this mechanism, the larger alkyl radicals either continue to decompose or are stabilized by abstracting hydrogens from other large alkanes. It has been found, however, that ethylene yields (ethylene is produced from radicals on the ends of the alkane chains) are too high from the simplest model. To correct this shortcoming, it is assumed in the complete RKH mechanism that all radicals with chain lengths greater than five internally isomerize (5). Several researchers have tested this modified mechanism and have found good agreement with experiment (7-11).

In this paper, a new kinetic model describing the pyrolysis of complex mixtures of hydrocarbons is presented. This free radical model is based on conventional elementary reaction steps and rate constants taken from the literature. The reactions which have been included, their rate constants, and literature references are listed in Table I.

In developing this hydrocarbon cracking model, we have extended the RKH model to higher temperatures. This has been accomplished by including mechanisms for the

decomposition of ethyl radical to ethylene (reaction 12), propyl radical to propylene (reactions 13 and 14), vinyl radical to acetylene (reaction 31); for hydrogen abstractions from all gas species by H radicals (reactions 32-37) and by larger radicals from both small and large molecules (reactions 38-48); and for additions to ethylene, propylene, and acetylene by H (reactions 12, 13, and 31) and to alkenes by CH_3 (reactions 15, 16, and 25). Rather than assuming that heavy radicals always isomerize before decomposition, we have also included isomerization rates (reactions 49 and 50) which are used to determine the extent of isomerization in competition with the other processes which can create or destroy large radicals.

Many of the rate constants used in the model have been taken unchanged from an excellent compilation by Allara and Shaw (12) and are the values used by Edelson and Allara (13) in their sensitivity analysis of propane and butane cracking. Some of these rate constants have been adjusted slightly for the following two reasons: 1) Adjustments were made within the reported error tolerances to make the model's predictions agree better with experiment. 2) Since these rate constants were collected to describe the pyrolysis of n-alkanes in the temperature range of 700-850 K, adjustments were made in the Arrhenius parameters to better fit higher temperature data while still maintaining the same rate at 775 K.

The constants for reactions 20-30, 44, and 46-48 were all adjusted to improve the distributions of high molecular weight hydrocarbons from the cracking of large alkanes. The hydrogen transfer rates are slightly higher than those of Allara and Shaw while the decomposition rates are slightly lower. The termination rate (reaction 11) is an adjustable parameter of the model and is described in more detail below. The rates for hydrogen abstractions from CH_4 (reactions 32 and 38-41) were calculated using the Allara and Shaw rate constants for the reverse reactions and thermochemical kinetics (14). The rate constants for additions of CH_3 to alkenes (reactions 15, 16, 20, and 25) were taken from Allara and Shaw and are values for the

formation of unbranched secondary radicals; the model does not permit the formation of branched hydrocarbons as the result of addition reactions. The forward rate of reaction 31 was taken from Westbrook, Dryer, and Schug (15) while the reverse rate was calculated using thermochemical kinetics (14). The rate for hydrogen abstractions from ethylene (forward reaction 35) is an Arrhenius approximation to the rate expression used by Westbrook, Dryer, and Schug (15) and is balanced by a reverse rate constant calculated using thermochemical kinetics (14).

The model needs as inputs the temperature-time profile for the reactor, initial concentrations, the pressure, and the integration step size. A standard kinetics file is used for all simulations. Outputs from the model are calculated time, temperature, gas concentrations (H_2, alkanes, alkenes, acetylene, and dienes), radical concentrations (H, alkyl, alkenyl and total) and radical reaction velocities for all the categories of reactions listed in Table I.

In the current model we have assumed a homogeneous reaction mixture. This is a fairly good assumption for an entrained flow reactor and for shock tube experiments, but is definitely a limitation for comparisons with other types of data. More accurate treatments of transport effects are being developed as part of our ongoing modeling efforts.

MODEL SOLUTION

Steady State Solution – The model is solved using a steady state (SS) approximation to calculate new radical populations at the start of each integration step in order to shorten the calculation time. According to Benson (16), steady state approximations are valid as long as radical populations are small relative to gas populations. This has been the case in all our simulations for temperatures up to 1500 K. The accuracy of the SS method has also been checked by comparing solutions

of simplified model problems, where many of the rate constants in Table I are set to zero, with exact integrations using Gear's method (17). It was found to give good agreement at temperatures up to 1800 K in test cases on ethane, ethylene and heptane pyrolysis models.

Single Termination Rate Constant - A second assumption was made to simplify the solution of the network of equations. This was to assume that all radicals in the simulation recombine with each other and they all react at the same rate (reaction 11). This linearizes the algebraic equations for the individual radical populations. Strictly speaking, this assumption is incorrect (12), since larger paraffinic radicals recombine at a slower rate (log A = 9.5) than do methyl radicals (log A = 10.4). In addition, radical disproportionations are not included in the mechanism at all. However, for conditions where the propagation steps are much faster than initiation and termination steps, reaction chains are long and relative product yields are independent of the termination mechanism (16). Absolute yields are fixed in these cases by the total radical population which is determined by the rates of radical creation (initiation) and destruction (termination). We, therefore, considered the termination rate constant used in reaction 11 to be a model fitting parameter which was varied to give the best absolute yields for our simulations. We have monitored the relative velocities of each type of reaction in our simulations and have concluded that, for temperatures less than 1500 K, the free radical chain reactions are long enough to minimize the errors introduced by the assumption of a single recombination rate. We have, however, developed a solution technique for non-linear radical equations which does not require this assumption in order to extend our model to higher temperatures. This version of the model will be reported on in a later paper. It confirms that the single termination rate assumption is generally good below 1500 K.

Radical Distributions for the Large Alkanes and Alkenes - One of the

difficulties associated with extending the RKH mechanism to describe the cracking of long chain length n-alkanes, is that increasing numbers of radicals must be included in the simulations. For example, radicals at the 1 positions of alkanes react differently than radicals at their 2 or 3 positions. (See reactions 13-30 of Table I.) Technically, separate radical populations should be kept for each position on each alkane and alkene included in the simulation. The number of differential equations which must be solved rapidly proliferates and becomes computationally unmanageable.

To avoid this problem, we have included one alkyl radical, PR_i, and one alkenyl radical, OR_i, for each hydrocarbon chain length, i, included in the simulation. The distributions of radicals over the various carbons in each of these species are given by normalized stoichiometric coefficients, Y_{ij} and Z_{ij}, where i is the number of carbons and j is the location on the chain. For example, the concentration of radicals on the 1 position of an alkyl radical with chain length 10, $1-PR_{10}$, is written in terms of a stoichiometric coefficient as $Y_{10,1} PR_{10}$. Given values for Y_{ij} and Z_{ij}, reactions 13-30 describe how the heavy alkyl and alkenyl radicals decompose. (In these equations O_i is an alkene of length i and D_i is a diene of length i.)

In the RKH mechanism the equivalent of Y_{ij} coefficients are calculated by: 1) statistically abstracting hydrogens from all available positions on the alkane and 2) assuming all radicals formed in step 1 isomerize through 6 member transition states. Since it is known that secondary hydrogens are more easily abstracted than primary, a weighting factor of $exp(2/RT)$ is used to determine the radical distribution between primary and secondary carbons. Similarly, a weighting factor of $exp(4/RT)$ is used to determine the redistribution of hydrogens during isomerization. A very lucid description of the calculation of Y_{ij} coefficients in the RKH model is presented in the appendix of Fabuss et al. (7).

The problems with the RKH method of calculating Y_{ij}'s are that: all radicals

are assumed to isomerize, only source terms are used to determine radical populations, and the relative velocities of the various types of radical reactions are not taken into account. In addition, the RKH method can not predict changes in the relative importance of reactions as temperatures are increased. For example, isomerization is always considered to be infinitely fast relative to decompositions regardless of the reaction temperature. To improve upon the RKH calculation, we have implemented a steady state solution for the Y_{ij} and Z_{ij} coefficients. This solution calculates values for the Y_{ij} and Z_{ij} coefficients by balancing the source and loss terms for each radical. These radical distributions can, therefore, change with reaction conditions and are different for each alkane or alkene in the simulation.

Summary of the Solution Procedure - The method of solving the kinetic equations of Table I is summarized in Fig. 1. Initial values of the gas concentrations, Y_{ij} and Z_{ij} coefficients, time (t), and temperature (T) are read into the program from a data file (Step 1). Next the steady state radical populations are calculated (Step 2) and are used to construct velocities for the gas concentrations (Step 3). New values of the radical stoichiometric coefficients are calculated in (Step 4) using current gas and radical concentrations. Finally, gas concentrations, time and temperature are updated in Step 5. The integration is continued by returning to the steady state calculation of radical populations in Step 2 until the ending time, t_f, is reached. The initial values of Y_{ij} and Z_{ij} are calculated by passing through Steps 2, 3, and 4 twenty times before concentrations are changed for the first time in Step 5. Our experience has been that once correct values of Y_{ij} and Z_{ij} are calculated at the beginning of a simulation they change very slowly as the gas concentrations are integrated.

If the model of Table I were solved exactly for a mixture of C_{20} alkanes, coupled stiff differential equations for 59 gases (H_2, 20 alkanes, 19 alkenes, and 19 dienes) and for 283 radicals (H, 110 alkyl, and 172 alkenyl) would have to be solved. The

assumptions of steady state conditions and a single termination rate constant reduce the problem to 59 coupled nonstiff differential equations for the gases, a quadratic equation for R_{total}, and solution of a system of 282 linear algebraic equations for the radicals. Introduction of the Y_{ij} and Z_{ij} coefficients further reduces the algebraic equations to a system of 40 linear equations for the radicals (H, 20 alkyl, 19 alkenyl) and iterative solution of 277 equations for the Y_{ij}'s and Z_{ij}'s. The net effect of all three approximations is an enormous decrease in computer run-times. The simulations presented in Figs. 3 and 4 for hexadecane and Solpar were each carried out in less than 40 minutes on a PDP 11/23 laboratory minicomputer.

COMPARISON OF MODEL WITH EXPERIMENTAL DATA

Extensive simulations were made of both in-house and literature data to test the model predictions. In this paper, selected results are presented for simulation of flow reactor data for pyrolysis of butane (1373 K, 1 atm), hexadecane (866-977 K, 68 atm) and Solpar (1053 K, 1 atm.) and of shock tube data for octane pyrolysis and hydropyrolysis (1000-1500 K).

Butane - Data for 1373 K butane pyrolysis was obtained in our laminar entrained flow reactor. These are compared with the model in Figs. 2a-f for the major gas species. This reactor has been discussed previously (18). It consists of a heat exchanger and test section contained in a furnace. An inert gas stream (N_2 or He) is preheated during transit through the heat exchanger, turns through a U-tube and enters a 5 cm diameter test section. The reactant is introduced into the test section at variable positions through a movable water cooled injector. The reacting stream passes optical access ports for an FT-IR beam shortly before being quenched in a water cooled collector. The pyrolysis results in Fig. 2 are plotted against the injector height above the optical port. The butane was fed at 2-3 g/min with about

1 g/min of nitrogen carrier (primary gas). Nitrogen (secondary gas) was fed to the heat exchanger at 27 standard liters/min to provide an averaged gas velocity of 1 m/s within the test section. The initial butane concentration (after complete mixing) was 2.4×10^{-4} moles/liter. The residence time was varied from 60 to 600 msec. The FT-IR allows data to be obtained on gas temperature and composition as discussed previously (18).

These simulations were done in two stages. First a heat transfer model was developed to predict the average gas temperature at the window. In general, the agreement with the FT-IR determined temperature was within 20°C. Next the heat transfer model was incorporated into the cracking model as a subroutine which provided an updated temperature after each time increment.

The agreement between the data and cracking model predictions in Fig. 2 is generally quite good, especially at the shorter injector distances. At longer distances, the secondary pyrolysis reactions (e.g., ethylene to acetylene and acetylene to benzene) become important. Based on Fig. 2a and the temperature model predictions, it appears that the overall cracking rate of butane is too high at temperatures above 1000°C. This point is discussed further below. The value of the termination rate constant used for these simulations was $\log_{10}A = 9.9$.

Hexadecane – In Fig. 3 results of simulations for the cracking of hexadecane at 68 atm. of pressure are presented. These are compared with the data of Fabass and co-workers (19). for carbon number distribution. A termination rate constant of $\log_{10} A = 10.9$ was used for these simulations. The residence times were chosen to make the experimental and theoretical extents of cracking agree. They differ slightly from the residence times calculated by Fabuss and co-workers (19): 5.8, 1.25, and 5.0 s for runs 23, 24, and 22 compared with 5.8, 2.3, and 6.5 reported in their paper. Apparently, at high extents of reaction our model slightly overpredicts the overall cracking rate of hexadecane, as it did for butane.
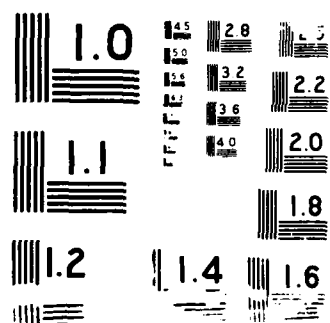
When compared at equal extents of reaction, the agreement between the theoretical and experimental product distributions is good: for low extents of reaction, both theory and experiment show relatively large concentrations of heavy alkanes and alkenes. As the cracking continues, the heavy hydrocarbons gradually disappear until, at 99.8% decomposition (Figs. 3e and f), the concentrations of alkanes and alkenes bigger than C_3's are almost negligible. For low extents of reaction, the experimental concentrations of C_5-C_8 alkanes are also slightly larger than for the other heavy alkanes. This behavior is partially reproduced by the simulations, although the exact shape of these curves is not predicted. Finally, for low extents of reaction, the experimental and theoretical methane yields are smaller than the ethane yields. However, as more high molecular weight hydrocarbons decompose, the methane yields increase and overtake the ethane yields.

Despite the close agreement between theory and experiment, there are several systematic discrepancies evident in Fig. 3. The yields of ethane are always too low; methane yields are reasonable for low extents of reaction but are too low for the later stages of decomposition; and as cracking proceeds, the yields of ethylene become too large while the yields of propylene become too small. We believe that these systematic errors are partially due to the fact that, in our model, large dienes are considered to be inert and are not allowed to crack into smaller gases. (This restriction was made in order to reduce the number of radical concentrations and stoichiometric coefficients in the model.) Therefore, any carbons contained in these large dienes are removed from the yields of other small gases such as methane or ethane.

Solpar - The gas phase cracking of mixtures of heavy alkanes can also be simulated using the mechanism of Table I. In Fig. 4, product distributions are presented for the cracking of Solpar, a commercial mixture of alkanes containing 8.2% C_{14}, 26.5% C_{15}, 21.9% C_{16}, and 13.7% C_{17} (20). These simulations were carried out

isothermally at 1053 K for residence times of 78, 117, and 192 ms. For these runs, the termination rate constant was $\log_{10} A = 9.7$. It can be seen that calculated product distributions are very close to those measured experimentally. In addition, the theoretical residence times are almost exactly the values calculated by Billaud and Freund (20). A slight discrepancy is evident, however, in the yields for propylene and possibly butene. As in the case of hexadecane cracking, these errors are probably due to the excessive formation of dienes.

Octane - In Fig. 5, data for major species from the shock tube pyrolysis of octane (Doolan and Mackie (21)) are compared with predictions from the hydrocarbon cracking model. The time for these simulations was 3.0 ms at the finish and the termination rate constant was $\log_{10} A = 10.9$. It can be seen that the onset of pyrolysis is correctly predicted and that the curve shapes are correct for most of the gases. The heights of the curves are also reasonable for product concentrations varying from 4.0×10^{-6} moles/liter up to 8.0×10^{-4} moles/liter. However, several disagreements between theory and experiment are also evident in these figures: 1) the concentration curve for octane falls off too rapidly at the higher temperatures; 2) acetylene, butadiene, and methane yields are underestimated at high temperatures. The latter model errors are worse at higher temperatures where a large portion of the octane has been consumed and there are appreciable concentrations of heavy alkenes and light gases such as methane, ethylene, propylene, and propane. This is the regime where the initial pyrolysis products begin to crack. These discrepancies at higher temperatures can probably be attributed to the model's treatment of the secondary pyrolysis reactions, which is incomplete at this stage. One group of reactions, which is missing from Table I and may be important is Diels-Alder additions. In these reactions ethylene and propylene are thought to react with dienes to form C_6 cyclic compounds (20,22) which are precursors for benzene, toluene, and soot. We are currently working to include some of these reactions in the

mechanism of Table I.

Doolan and Mackie also collected shock tube data for the hydropyrolysis of octane in a 50:50 atmosphere of Ar and H_2 (21). Their data and our simulations are shown in Fig. 6. Once again the onset of pyrolysis is correctly predicted, the curve shapes are reasonable, and overall product yields are fairly accurate over two orders of magnitude in concentration. However, similar discrepancies as in the pyrolysis case are observed at the higher temperatures.

Cracking of Octane with Modified Rate Constants - From the comparisons of data and simulations in Figs. 2-6, it was found that consumption of heavy alkanes and alkenes is too fast at the higher temperatures. The simulations in Figs. 2-6 used rate constants which were either given in Allara and Shaw or were very slightly modified from their values. Since their rate constants are supposed to be valid at 700-800 K, it is not surprising that they are in error at temperatures as high as 1470 K. It seems reasonable to require that all the rate constants altered to better fit experiments should also equal the Allara and Shaw rates at 700 K, i.e., changes in the activation energies are coupled to changes in the frequency factors so that the rates at 700 K are fixed.

Analysis of the rate of formation and loss of octyl radicals has shown that, at 1400 K under shock tube conditions, octane is mainly lost by initiation reactions and not by hydrogen abstractions. The too rapid rate of cracking observed in our simulations could, therefore, be due to an error in the initiation rates for large alkanes (reactions 5 and 6). When these rate constants were reduced in size at 1400 K ($\log_{10} A_5$ = 15.9, E_5 = 82.3; $\log_{10} A_6$ = 15.1, E_6 = 76.3), dramatically better experimental fits for octane cracking were obtained, as shown in Fig. 7. The resulting rates agree with the Allara and Shaw values at 700 K but are about four times slower at 1400 K. They are very close to the values reported by Doolan and Mackie (21) for their modeling of this shock tube data ($\log_{10} A$ = 15.3, E = 77.6).

Improved results were also obtained for butane pyrolysis at 1373 K. However, it was found that if these same changes were made for the lower temperature cracking experiments (hexadecane and Solpar) the overall rate was too high at the lowest temperatures. Consequently, further adjustment and comparisons with additional data will be required to fix these values.

In the new simulations (Fig. 7), the termination rate constant giving the best result was $\log_{10} A = 10.1$, which is also closer to the value for CH_3 radical ($\log_{10} A = 10.3$). We are continuing our efforts to identify and adjust the key rate constants of Table I in order to obtain better fits for experimental data at high temperatures and high extents of reaction.

CONCLUSIONS

Based upon the simulations discussed in this paper, it appears that the model of Table I is a valid extension of the RKH mechanism to higher temperatures and higher extents of reaction. The cracking of butane at 1373 K was well predicted (Fig. 2). The high pressure cracking of hexadecane was accurately simulated over the temperature range 866-977 K with up to 80% cracking (Fig. 3). The cracking of a complex mixture of $C_{14}-C_{17}$ alkanes at 1053 K was also predicted for high extents of reactions (Fig. 4). In addition, simulations for the shock tube pyrolysis and hydropyrolysis of octane are reasonably accurate up to approximately 1400 K (Figs. 5-7). We, therefore, conclude that 1) the mechanism used to treat the initial pyrolysis of high molecular weight alkanes is correct and 2) simulations for the cracking of mixtures of n-alkanes (containing up to twenty carbons) should be accurate at temperatures up to approximately 1400 K.

Several model deficiencies are also apparent in these simulations: 1) the overall cracking rate is too high above 1000 K; 2) the mechanisms for the creation

C-16

and loss of dienes are either incomplete or the rate constants are in error; and 3) additional reactions for ethylene and acetylene pyrolysis are needed at high extents of reaction.

NOMENCLATURE

R - alkyl or alkenyl groups or radicals

P_i - an alkane of chain length i

O_i - an alkene of chain length i

D_i - a diene of chain length i

PR_i - the group of alkyl radicals with chain length i

OR_i - the group of alkenyl radicals with chain length i

$j-PR_i$ - a radical at the jth position of an alkane with chain length i

$j-OR_i$ - a radical at the jth position of an alkene with chain length i

$s-PR_i$ - the group of radicals on the secondary carbons of an alkane with chain length i

Y_{ij} - the fraction of radicals on an alkane with chain length i which are found on the jth carbon

Z_{ij} - the fraction of radicals on an alkene with chain length i which are found on the jth carbon

R_{total} - the total concentration of radicals in the model

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TABLE I. THE HYDROCARBON CRACKING MODEL

TABLE I. THE HYDROCARBON CRACKING MODEL

$$k = A \exp(-A/RT), \text{ Units} = (\ell, \text{ sec, moles, kcal})$$

REACTION	FORWARD RATE		REVERSE RATE		REF.
	log A	E	log A	E	
Initiation:					
1. $C_2H_6 \longrightarrow CH_3 + CH_3$	16.7	89.0	-	-	12
2. $C_3H_8 \longrightarrow CH_3 + C_2H_5$	16.9	85.1	-	-	12
3. $C_4H_{10} \longrightarrow CH_3 + C_3H_7$	17.5	85.7	-	-	12
4. $C_4H_{10} \longrightarrow C_2H_5 + C_2H_5$	16.4	82.1	-	-	12
5. $RCH_3 \longrightarrow R + CH_3 \ (R > C_3H_7)$	16.8	85.4	-	-	12
6. $RR' \longrightarrow R + R' \ (RR' > C_4H_{10}, R' > CH_3)$	16.8	81.9	-	-	12
7. $C_4H_8 \longrightarrow C_3H_5 + CH_3$	16.1	73.4	-	-	12
8. $C_5H_{10} \longrightarrow C_3H_5 + C_2H_5$	16.0	71.4	-	-	12
9. $RC_3H_5 \longrightarrow R + C_3H_5 \ (R > C_2H_5)$	16.4	71.1	-	-	12
10. $(C_3H_5)_2 \longrightarrow C_3H_5 + C_3H_5$	14.4	59.4	-	-	12
Termination:					
11. $R + R' \longrightarrow RR' \ (R, R' \text{ any radicals})$	9.8	0	-	-	**
Decompositions and Additions:					
12. $C_2H_5 \rightleftharpoons C_2H_4 + H$	13.6	40.5	10.6	2.6	12
13. $2\text{-}C_3H_7 \rightleftharpoons C_3H_6 + H$	13.9	40.4	9.9	1.2	12
14. $1\text{-}C_3H_7 \rightleftharpoons C_3H_6 + H$	13.2	38.6	9.9	2.9	12
15. $1\text{-}C_3H_7 \rightleftharpoons C_2H_4 + CH_3$	13.1	32.5	8.1	7.7	12
16. $2\text{-}C_4H_9 \rightleftharpoons C_3H_6 + CH_3$	14.3	33.2	8.5	9.1	12
17. $1\text{-}C_4H_9 \longrightarrow C_2H_4 + C_2H_5$	13.4	28.8	-	-	12
18. $1\text{-}C_5H_{11} \longrightarrow C_2H_4 + C_3H_7$	13.5	28.4	-	-	12
19. $2\text{-}C_5H_{11} \longrightarrow C_3H_6 + C_2H_5$	12.7	29.1	-	-	12
20. $3\text{-}C_5H_{11} \rightleftharpoons C_4H_8 + CH_3$	14.2	33.0	8.3	8.9	12
21. $1\text{-}PR_i \longrightarrow C_2H_4 + 1\text{-}PR_{i-2}, \ i \geq 6$	12.8	30.0	-	-	12*
22. $1\text{-}OR_i \longrightarrow C_2H_4 + (1\text{-}2)\text{-}OR_{i-2}, \ i \geq 5$	12.8	30.0	-	-	12*
23. $2\text{-}PR_i \longrightarrow C_3H_6 + 1\text{-}PR_{i-3}, \ i \geq 6$	12.9	28.8	-	-	12*
24. $(i\text{-}1)\text{-}OR_i \longrightarrow C_3H_6 + (i\text{-}3)\text{-}OR_{i-3}, \ i \geq 6$	12.9	28.8	-	-	12*
25. $3\text{-}PR_i \rightleftharpoons O_{i-1} + CH_3, \ i \geq 6$	13.1	28.8	8.3	8.9	12*
26. $(i\text{-}2)\text{-}OR_i \longrightarrow D_{i-1} + CH_3, \ i \geq 5$	13.1	28.8	-	-	12*
27. $j\text{-}PR_i \longrightarrow O_{j+1} + 1\text{-}PR_{i-j-1}, \ i \geq 6, \ 3 \leq j \leq i-3$	13.1	28.3	-	-	12*
28. $j\text{-}OR_i \longrightarrow D_{j+1} + 1\text{-}PR_{i-j-1}, \ i \geq 6, \ 3 \leq j \leq i-3$	13.1	28.3	-	-	12*
29. $j\text{-}PR_i \longrightarrow O_{i-j+2} + 1\text{-}PR_{j-2}, \ i \geq 6, \ 4 \leq j \leq i-2$	13.1	28.3	-	-	12*
30. $j\text{-}OR_i \longrightarrow D_{i-j+2} + (j\text{-}2)\text{-}OR_{j-2}, \ i \geq 7, \ 5 \leq j \leq i-2$	13.1	28.3	-	-	12*
31. $C_2H_3 + M \rightleftharpoons C_2H_2 + M + H$	11.9	31.5	9.0	-6.5	14,15
Hydrogen Transfers:					
32. $H + CH_4 \rightleftharpoons H_2 + CH_3$	10.4	11.4	9.2	11.3	12,14
33. $H + C_2H_6 \rightleftharpoons H_2 + C_2H_5$	11.1	9.7	9.6	14.0	12
34. $H + C_3H_8 \rightleftharpoons H_2 + C_3H_7$	10.8	7.7	9.2	15.4	12
35. $H + C_2H_4 \rightleftharpoons H_2 + C_2H_3$	11.3	10.9	9.6	6.4	14,15
36. $H + C_3H_6 \rightleftharpoons H_2 + C_3H_5$	11.0	3.5	10.5	19.7	12
37. $H + RH \rightleftharpoons H_2 + R \ (R > C_3H_7 \text{ or } C_3H_5)$	11.1	7.7	9.5	15.7	12
38. $CH_3 + C_2H_6 \rightleftharpoons CH_4 + C_2H_5$	8.8	11.6	8.9	17.8	12,14
39. $CH_3 + C_3H_8 \rightleftharpoons CH_4 + C_3H_7$	8.8	10.5	9.1	20.9	12,14
40. $CH_3 + C_3H_6 \rightleftharpoons CH_4 + C_3H_5$	8.0	8.8	9.2	25.8	12,14
41. $CH_3 + RH \rightleftharpoons CH_4 + R \ (R > C_3H_7 \text{ or } C_3H_5)$	8.6	9.6	9.1	18.3	12,14
42. $C_2H_5 + C_3H_8 \rightleftharpoons C_2H_6 + C_3H_7$	7.7	10.4	8.5	12.3	12
43. $C_2H_5 + C_3H_6 \rightleftharpoons C_2H_6 + C_3H_5$	8.0	9.8	8.9	20.5	12
44. $C_2H_5 + RH \rightleftharpoons C_2H_6 + R \ (R > C_3H_7 \text{ or } C_3H_5)$	8.2	10.4	8.7	12.3	12*
45. $C_3H_7 + C_3H_6 \rightleftharpoons C_3H_8 + C_3H_5$	8.0	9.8	8.3	16.1	12
46. $C_3H_7 + RH \rightleftharpoons C_3H_8 + R \ (R > C_3H_7 \text{ or } C_3H_5)$	8.2	10.4	8.2	10.4	12*
47. $C_3H_5 + RH \rightleftharpoons C_3H_6 + R \ (R > C_3H_7 \text{ or } C_3H_5)$	8.7	16.4	8.2	9.8	12*
48. $R + R'H \longrightarrow RH + R' \ (R, R' > C_3H_7 \text{ or } C_3H_5)$	8.6	10.4	-	-	12*
Isomerizations:					
49. $s\text{-}PR_i \rightleftharpoons 1\text{-}PR_i \ (i \geq 5, \geq 5 \text{ member t.s.})$	11.1	23.4	11.0	20.0	12
50. $s\text{-}PR_i \rightleftharpoons 1\text{-}PR_i \ (i \geq 6, \geq 6 \text{ member t.s.})$	9.3	14.5	9.2	11.1	12

* Rate constants from Ref. 12 were slightly modified to improve fits of high temperature data.

** an adjustable parameter of the model
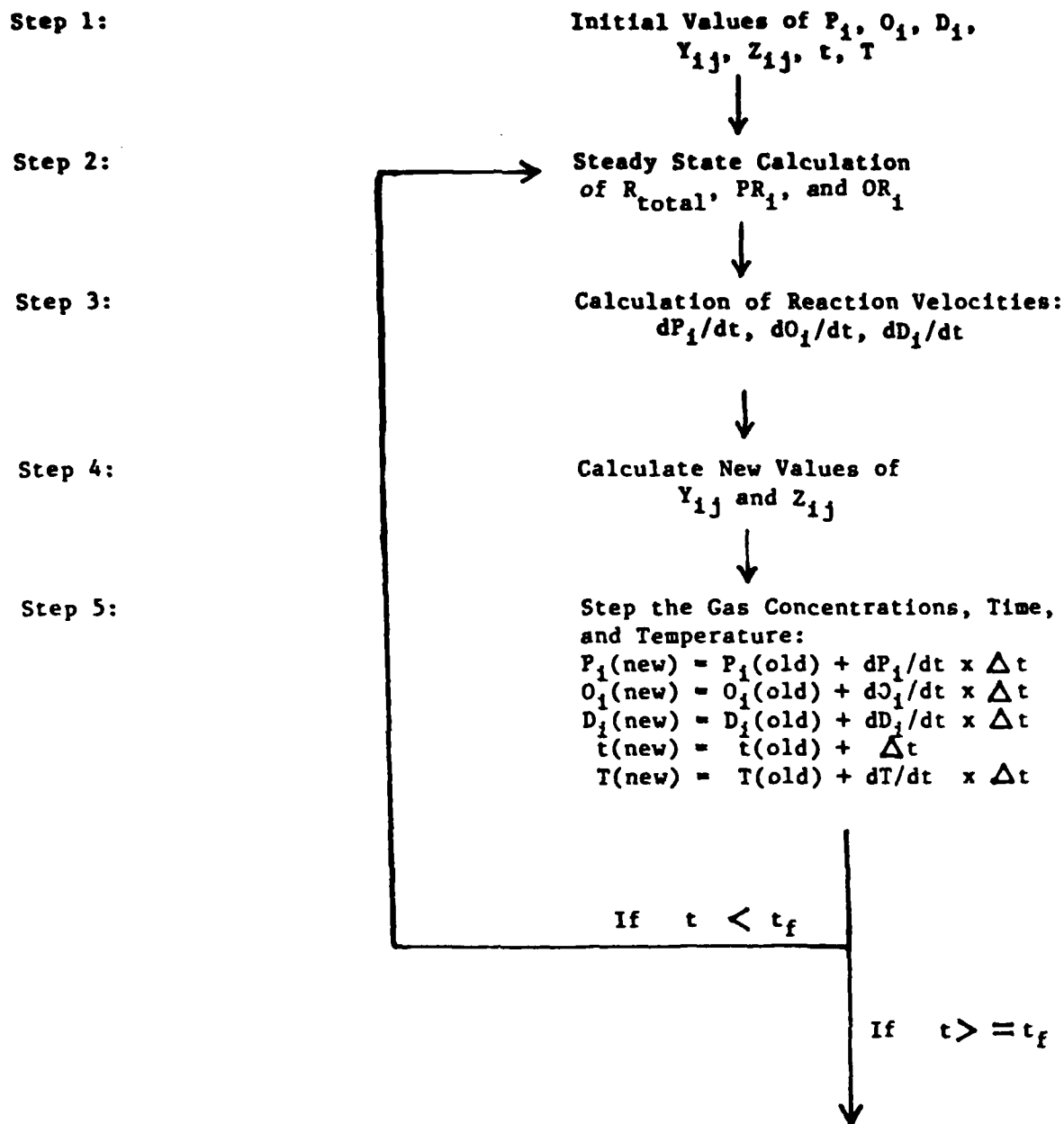
FIGURE CAPTIONS

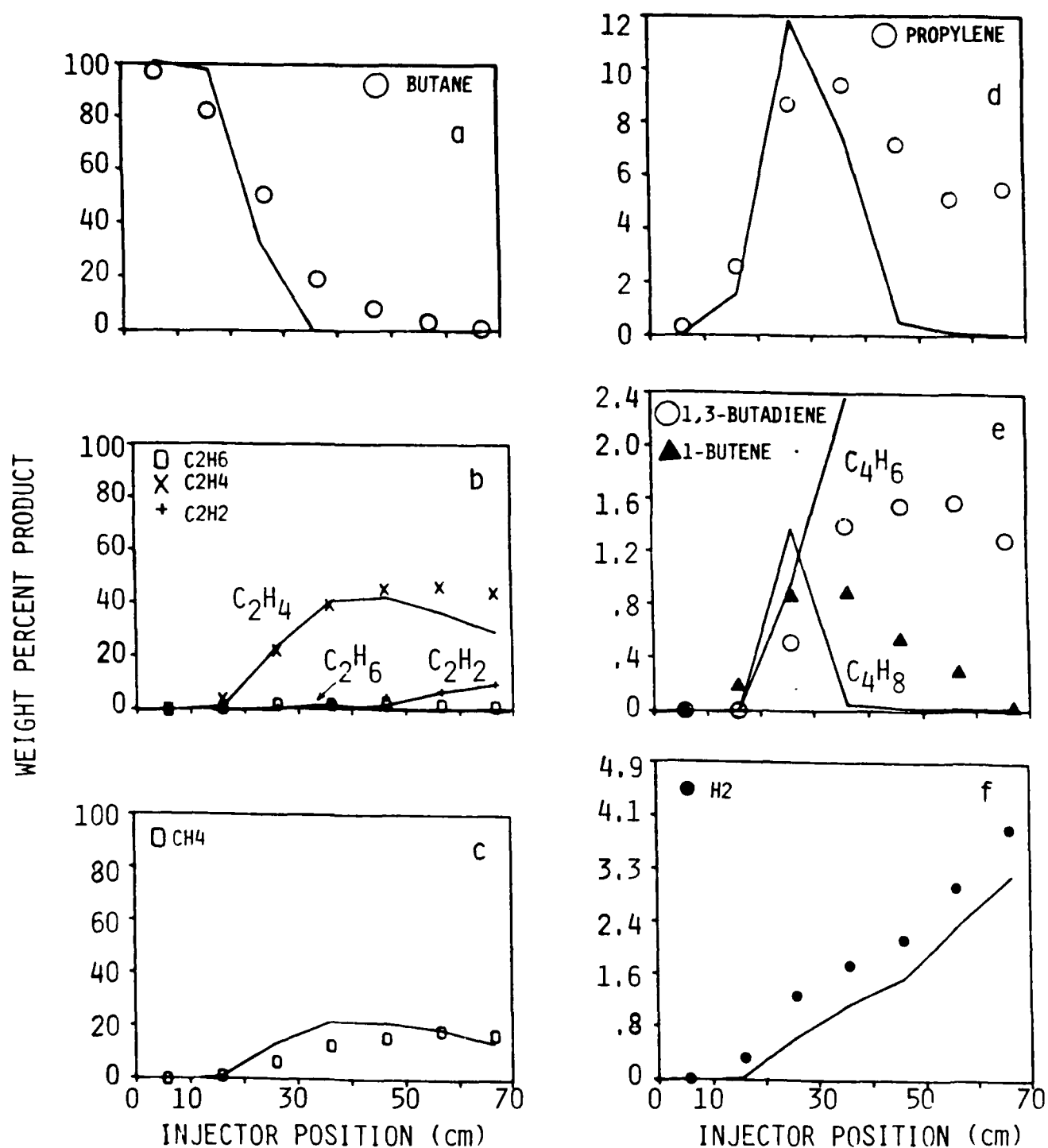Figure 1. Solution Procedure for Hydrocarbon Cracking Model.

Figure 2. Product Composition Profiles for Butane Pyrolysis in an Entrained
Flow Reactor at a Maximum Furnace Temperature of 1373 K. Solid Lines
are Model Predictions. Symbols are Experimental Data. Conditions:
Nitrogen Carrier, Average Gas Velocity = 1 m/sec, Pressure = 1 atm,
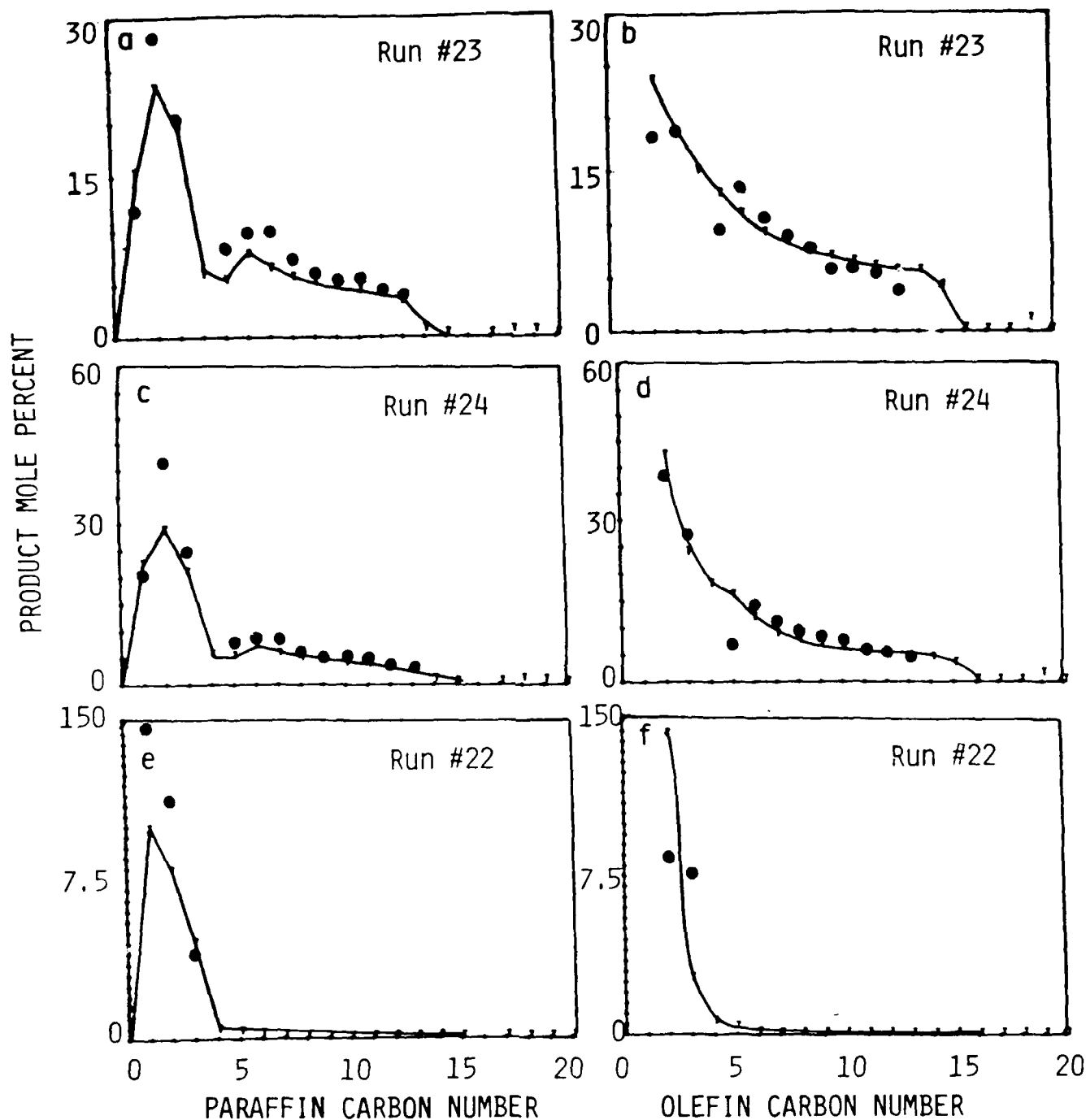Concentration = 2.4 x 10^{-4} moles/liter.

Figure 3. Paraffin and Olefin Carbon Number Distribution from the Thermal
Cracking of Hexadecane at 68 atm. (19). Symbols: (•) –
Experimental Data; (T) – Predictions of Cracking Model. Solid Lines
Connect Model Predictions. Experimental Conditions:
Run #22 – Temp. = 977 K, Time = 6.5 s, Amount Cracked = 97.1 wt%;
Run #23 – Temp. = 866 K, Time = 5.83 s, Amount Cracked = 29.6 wt%;
Run #24 – Temp. = 922 K, Time = 2.3 s, Amount Cracked = 41.6 wt%.
The Predicted Amounts Cracked were 99.8, 30.7 and 43.6 wt%,
Respectively. The Residence Times used for the Simulations were 5.0,
5.8, and 1.25 s, Respectively.

Figure 4. Paraffin and Olefin Carbon Number Distribution from the Thermal
Cracking of Solpar (A Commercial Mixture of C_{12} – C_{18} n-alkanes).
Symbols: (•) – Experimental Data from Ref. 20; (T) – Prediction of
Cracking Model. Solid Lines Connect Model Predictions. Experimental
Conditions: Run #1 – Temp. = 1053 K, Time = 80 ms, Amount Cracked =
75.8 wt%; Run #2 – Temp. = 1053 K, Time = 108 ms, Amount Cracked =
75.8 wt%. Run #3 – Temp. = 1053 K, Time = 188 ms, Amount Cracked =
92.8 wt%. The Residence Times Input to the Model were 78, 117, and
192 ms, Respectively. All runs were done in Steam at Slightly above
1 atm. Pressure.

Figure 5. Product Composition Profiles for Shock-Tube Pyrolysis of Octane.
Symbols: (E) – Experimental Data from Ref. 21; (T) – Predictions
of Cracking Model. Solid Lines Connect Model Predictions.
Experimental Conditions: Time = 3 ms, Initial Concentration =
3.3 x 10^{-4} Moles/Liter in Argon.

Figure 6. Product Composition Profiles for Shock-Tube Hydropyrolysis of Octane
in 50 Mole % H_2. Symbols: (E) – Experimental Data from Ref. 21;
(T) – Predictions of Cracking Model. Solid Lines Connect Model
Predictions. Experimental Conditions: Time = 3 ms, Initial
Concentration = 3.3 x 10^{-4} Moles/Liter in 50/50 Argon/H_2.

Figure 7. Product Composition Profiles for Shock-Tube Pyrolysis of Octane Using
Modified Initiation Rates. Symbols: (E) – Experimental Data from
Ref. 21; (T) – Predictions of Cracking Model. Solid Lines Connect
Model Predictions. Experimental Conditions: Time = 3 ms, Initial
Concentration = 3.3 x 10^{-4} Moles/Liter in Argon.

Step 1: Initial Values of P_i, O_i, D_i, Y_{ij}, Z_{ij}, t, T

Step 2: Steady State Calculation of R_{total}, PR_i, and OR_i

Step 3: Calculation of Reaction Velocities: dP_i/dt, dO_i/dt, dD_i/dt

Step 4: Calculate New Values of Y_{ij} and Z_{ij}

Step 5: Step the Gas Concentrations, Time, and Temperature:
$P_i(new) = P_i(old) + dP_i/dt \times \Delta t$
$O_i(new) = O_i(old) + dO_i/dt \times \Delta t$
$D_i(new) = D_i(old) + dD_i/dt \times \Delta t$
$t(new) = t(old) + \Delta t$
$T(new) = T(old) + dT/dt \times \Delta t$

If $t < t_f$

If $t >= t_f$

Figure 1. Solution Procedure for Hydrocarbon Cracking Model.

Figure 2. Product Composition Profiles for Butane Pyrolysis in an Entrained
Flow Reactor at a Maximum Furnace Temperature of 1373 K. Solid Lines
are Model Predictions. Symbols are Experimental Data. Conditions:
Nitrogen Carrier, Average Gas Velocity = 1 m/sec, Pressure = 1 atm,
Concentration = 2.4 x 10^{-4} moles/liter.

Figure 3. Paraffin and Olefin Carbon Number Distribution from the Thermal Cracking of Hexadecane at 68 atm. (19). Symbols: (●) – Experimental Data; (T) – Predictions of Cracking Model. Solid Lines Connect Model Predictions. Experimental Conditions:
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The Predicted Amounts Cracked were 99.8, 30.7 and 43.6 wt%, Respectively. The Residence Times used for the Simulations were 5.0, 5.9, and 1.25 s, Respectively.

Figure 4. Paraffin and Olefin Carbon Number Distribution from the Thermal Cracking of Solpar (A Commercial Mixture of C_{12} - C_{18} n-alkanes). Symbols: (•) - Experimental Data from Ref. 20; (T) - Prediction of Cracking Model. Solid Lines Connect Model Predictions. Experimental Conditions: Run #1 - Temp. = 1053 K, Time = 80 ms, Amount Cracked = 75.8 wt%; Run #2 - Temp. = 1053 K, Time = 108 ms, Amount Cracked = 75.8 wt%. Run #3 - Temp. = 1053 K, Time = 188 ms, Amount Cracked = 92.8 wt%. The Residence Times Input to the Model were 78, 117, and 192 ms, Respectively. All runs were done in Steam at Slightly above 1 atm. Pressure.
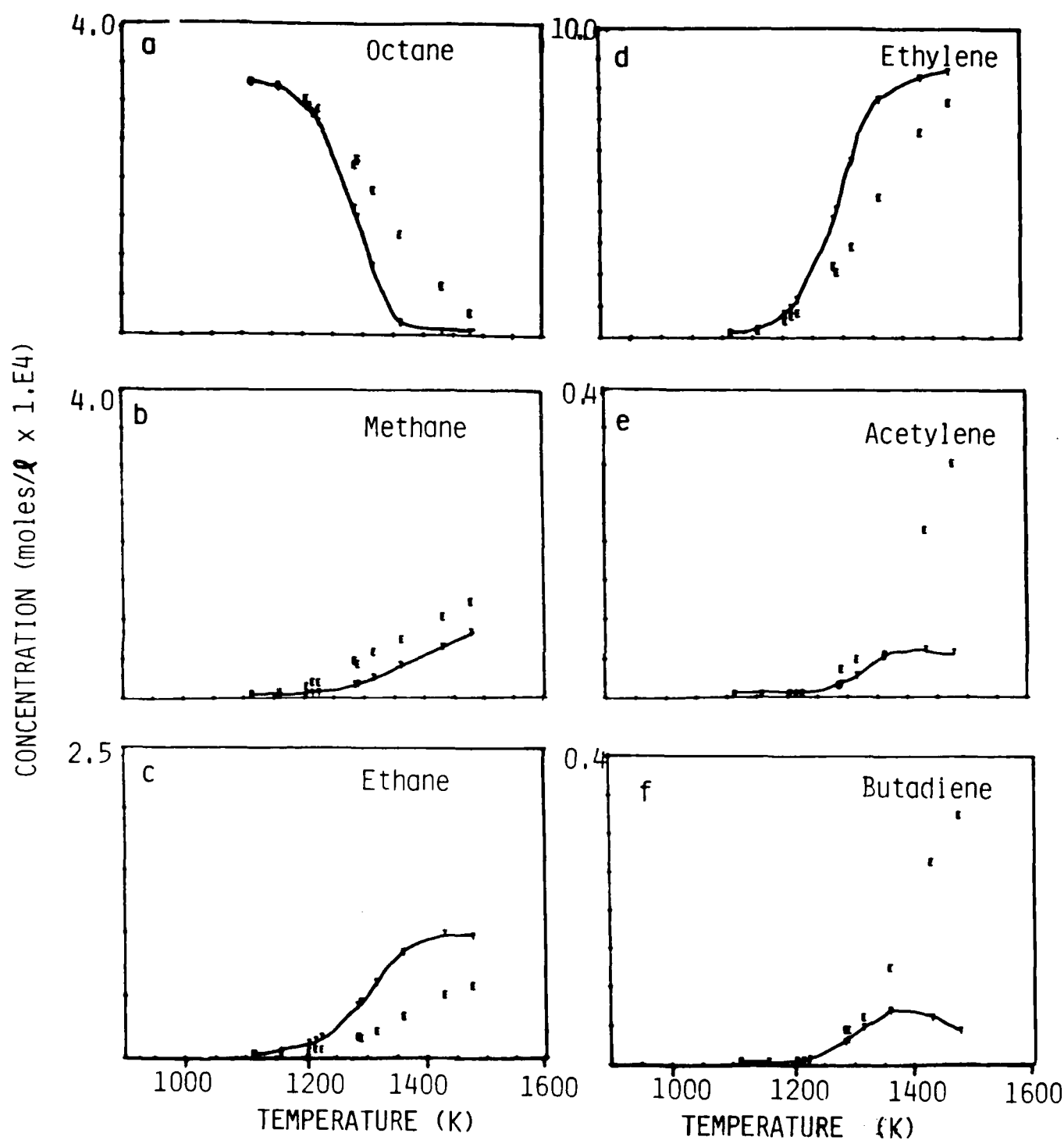
Figure 5. Product Composition Profiles for Shock-Tube Pyrolysis of Octane.
Symbols: (E) - Experimental Data from Ref. 21; (T) - Predictions
of Cracking Model. Solid Lines Connect Model Predictions.
Experimental Conditions: Time = 3 ms, Initial Concentration =
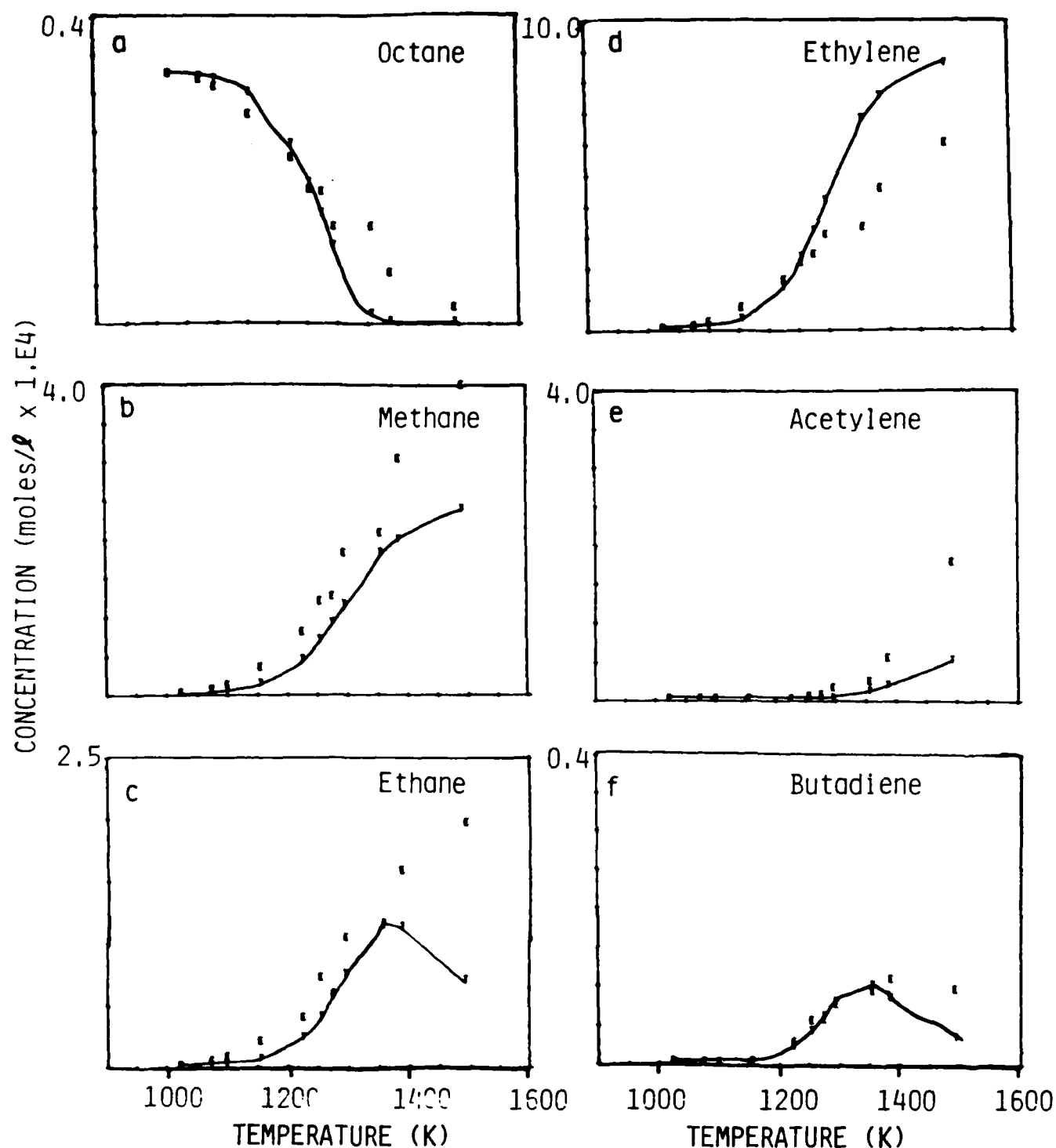3.3×10^{-4} Moles/Liter in Argon.

Figure 6. Product Composition Profiles for Shock-Tube Hydropyrolysis of Octane in 50 Mole % H_2. Symbols: (E) — Experimental Data from Ref. 21; (T) — Predictions of Cracking Model. Solid Lines Connect Model Predictions. Experimental Conditions: Time = 3 ms, Initial Concentration = 3.3 x 10^{-4} Moles/Liter in 50/50 Argon/H_2.
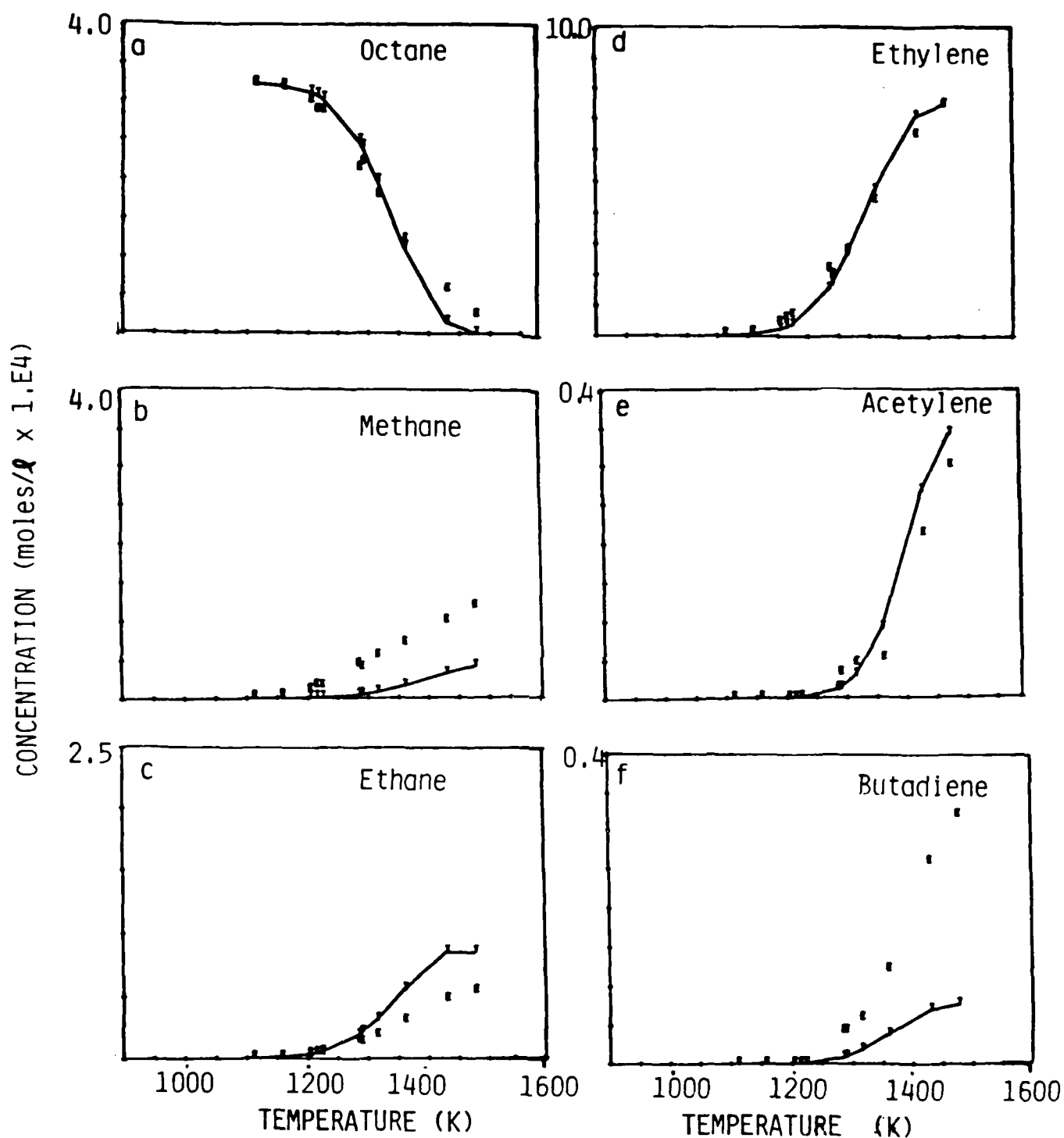
Figure 7. Product Composition Profiles for Shock-Tube Pyrolysis of Octane Using Modified Initiation Rates. Symbols: (E) - Experimental Data from Ref. 21; (T) - Predictions of Cracking Model. Solid Lines Connect Model Predictions. Experimental Conditions: Time = 3 ms, Initial Concentration = 3.3 x 10^{-4} Moles/Liter in Argon.

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